



FIG. 1

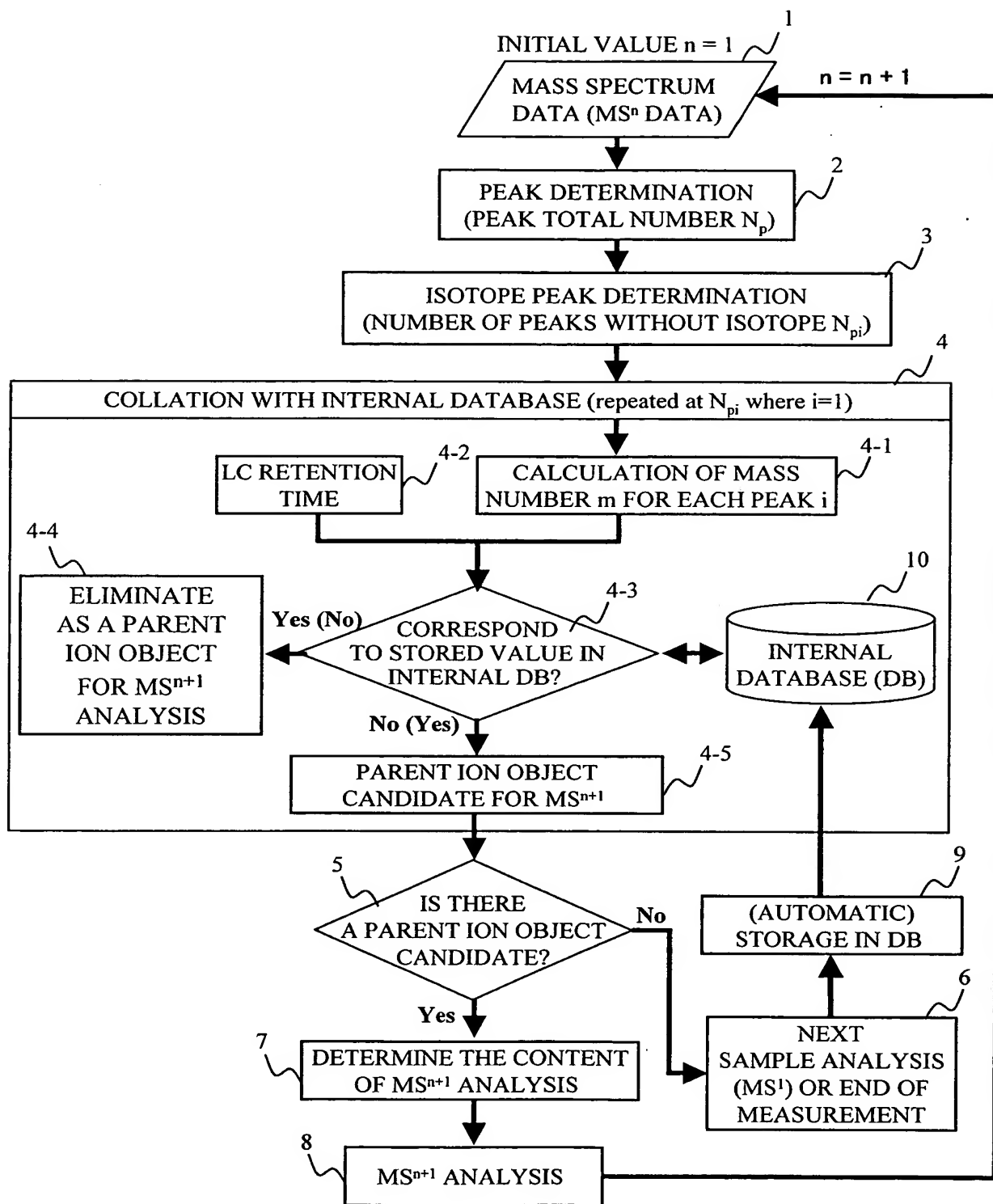


FIG. 2

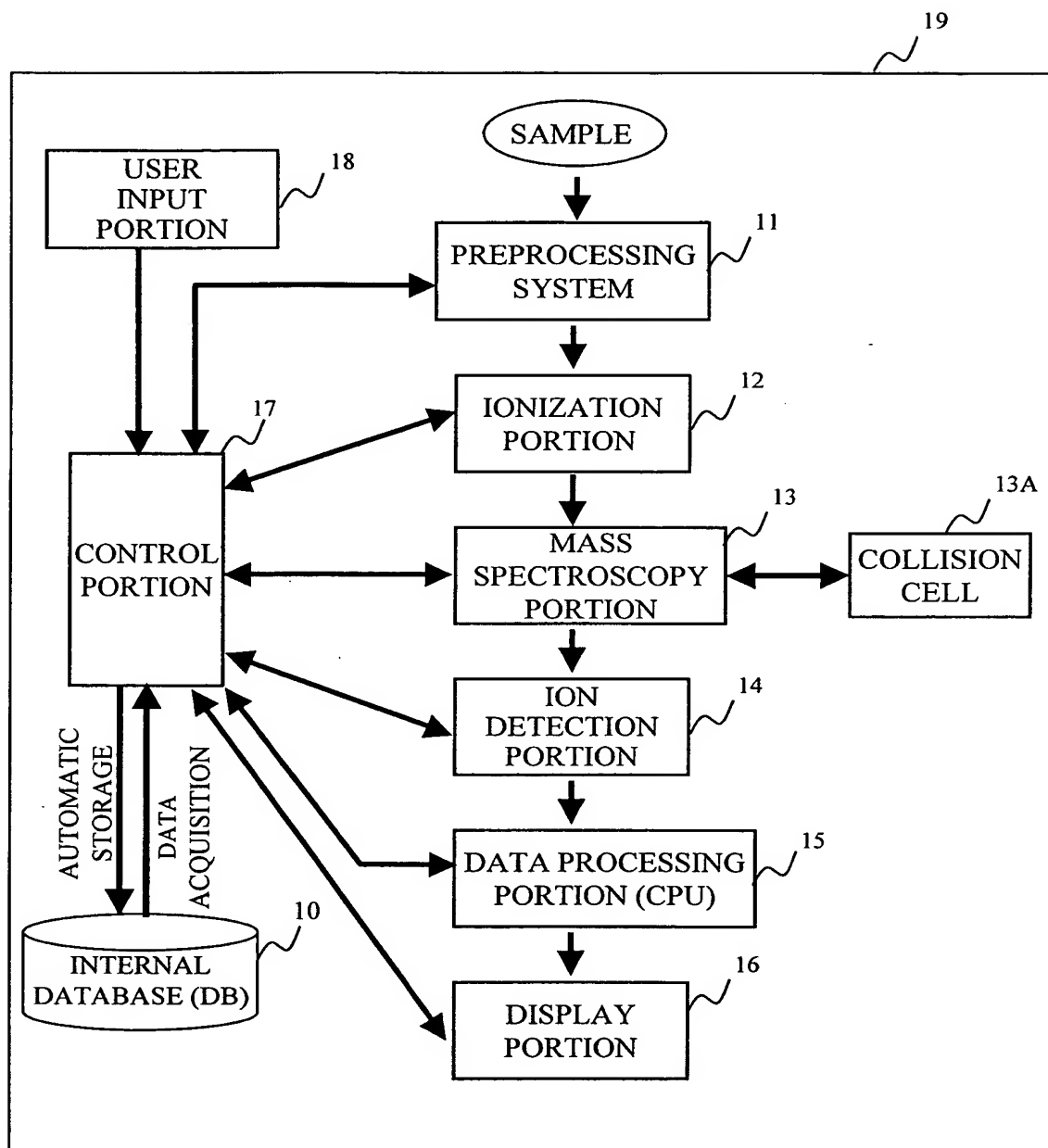


FIG. 3 A

PRIOR ART METHOD

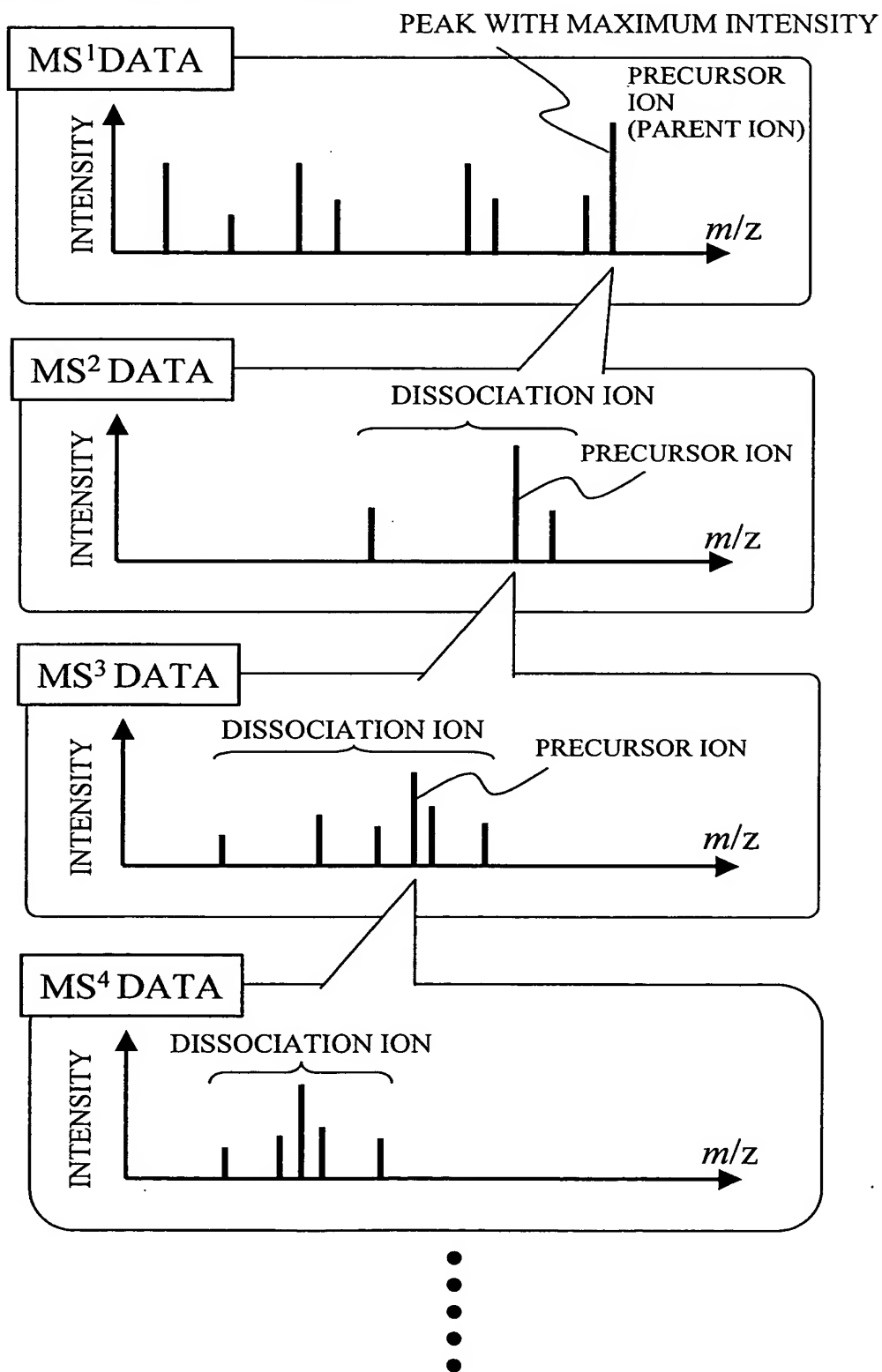


FIG. 3 B

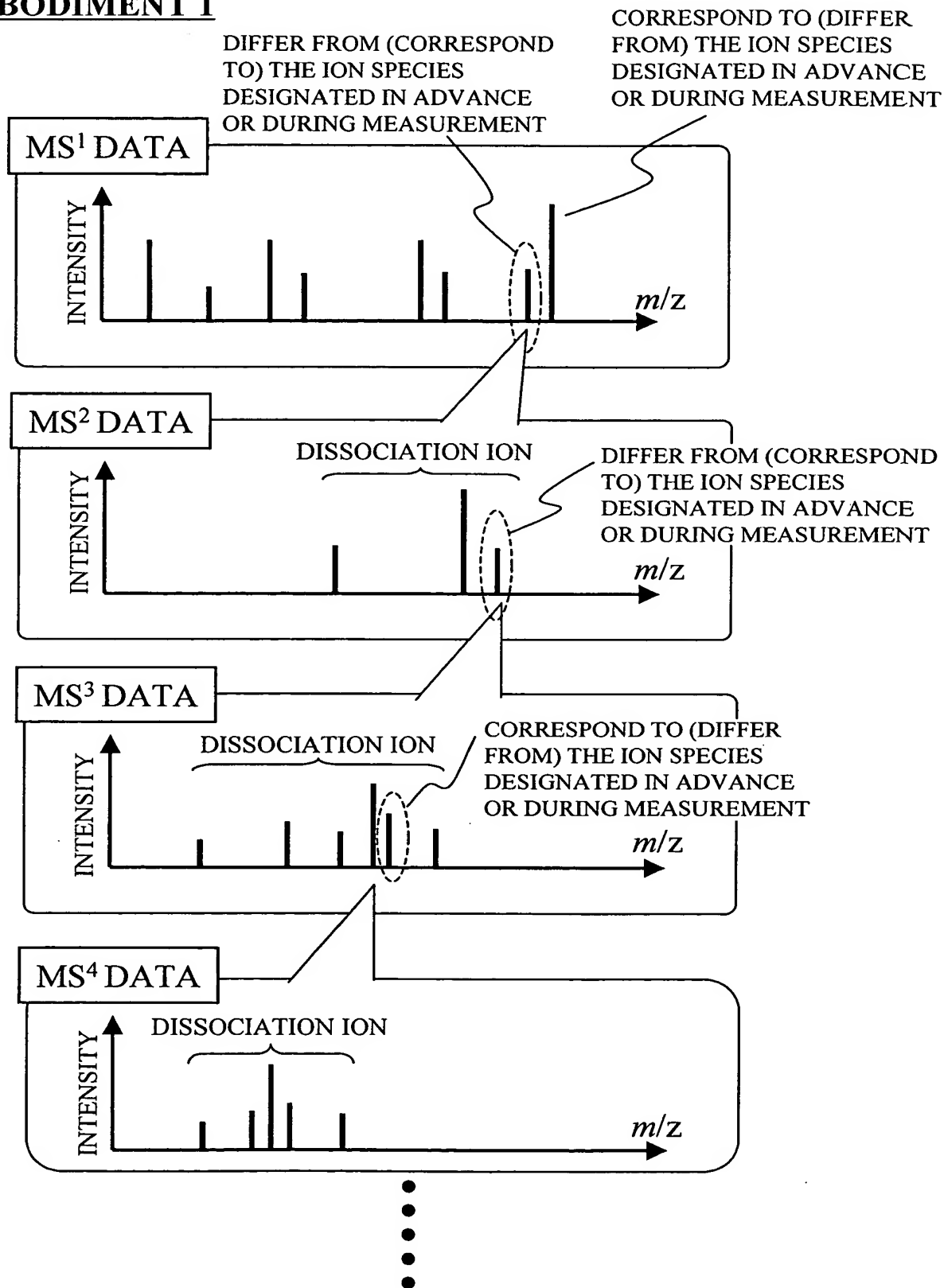
EMBODIMENT 1

FIG. 3 C

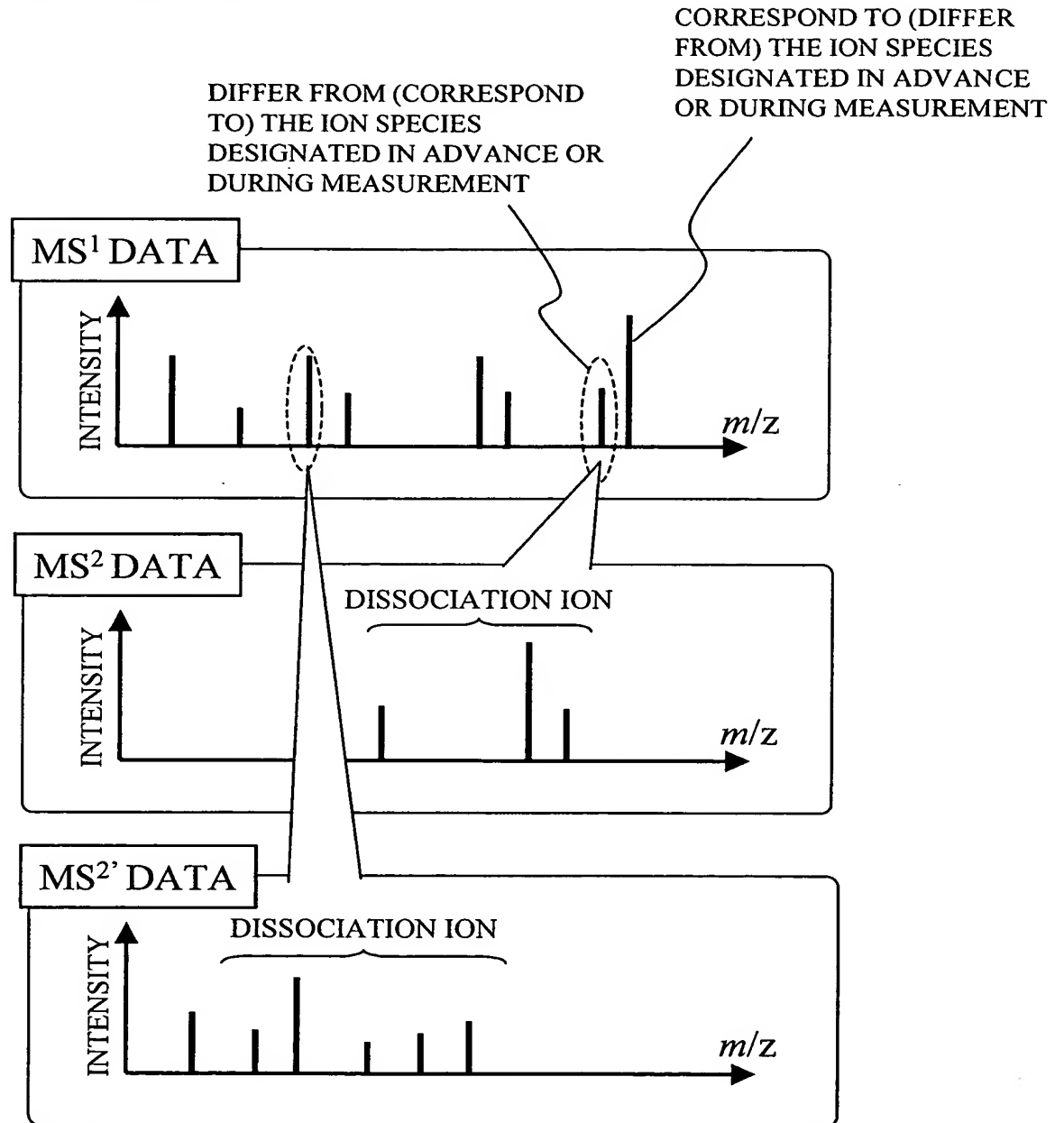
EMBODIMENT 2

FIG. 4

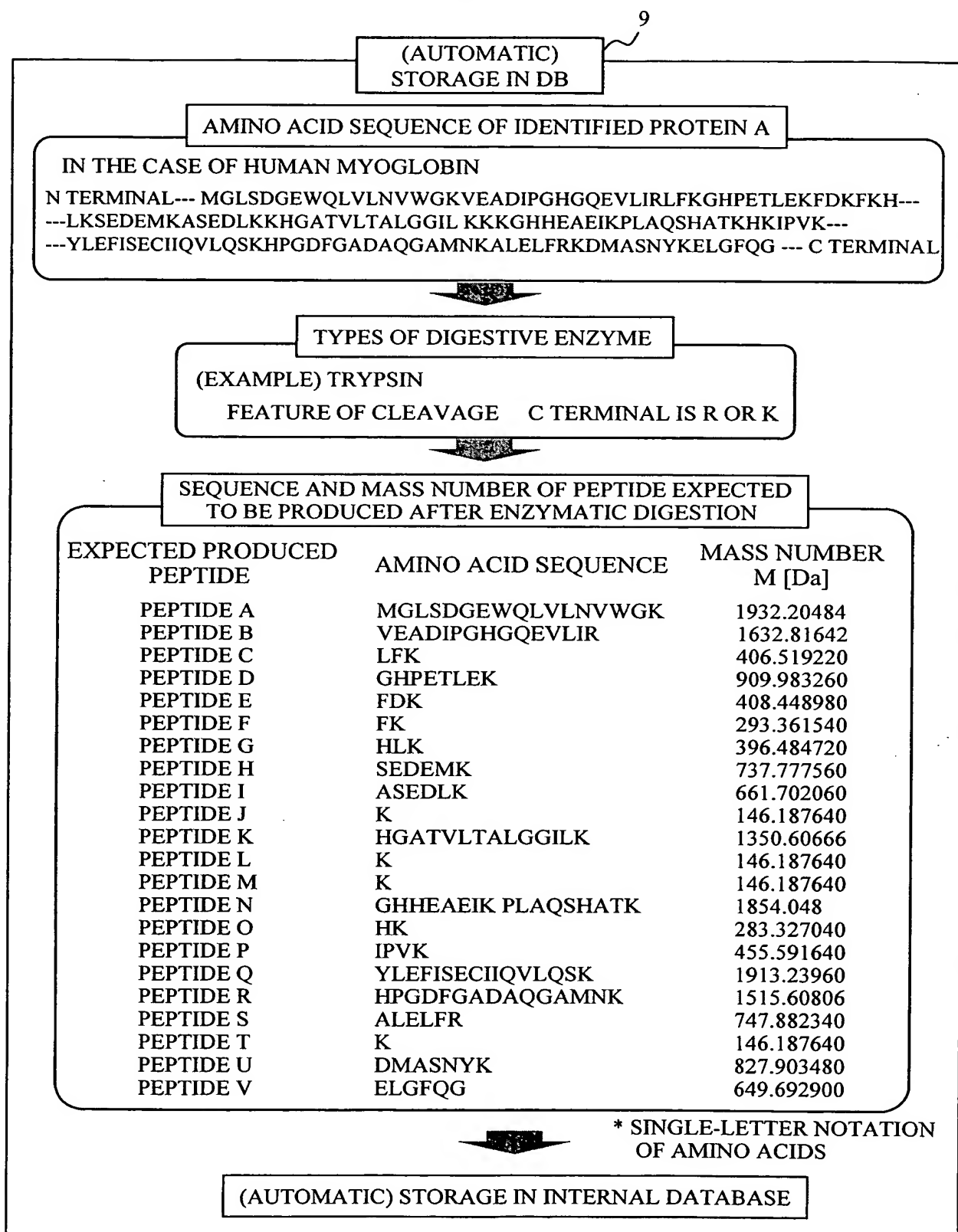


FIG. 5

10

INTERNAL DATABASE (DB)

CONTENT OF THE INTERNAL DATABASE

- CHARACTERISTICS DATA OF A PEPTIDE THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
(MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

PEPTIDE NAME /SEQUENCE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
PEPTIDE A	200	1	200	15160	20	2
PEPTIDE B	700	2	350	2100	28	3
PEPTIDE C	450	1	450	4754	35	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A PEPTIDE DERIVED FROM A PROTEIN THAT HAS ONCE BEEN IDENTIFIED OR THAT SHOULD BE ELIMINATED FROM THE OBJECTS FOR TANDEM ANALYSIS
(PROTEIN NUMBER, ID NUMBER, MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

PEPTIDE NAME /SEQUENCE	PROTEIN NAME	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
PEPTIDE A	PROTEIN A	570	1	570	25010	25	2
PEPTIDE B	PROTEIN A	652	1	652	3140	32	3
PEPTIDE C	PROTEIN A	652	2	326	58754	45	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
PEPTIDE D	PROTEIN B	1042	2	521	6456	22	2
PEPTIDE E	PROTEIN B	718	2	359	3080	35	3
PEPTIDE F	PROTEIN B	671	2	335.5	8054	48	3
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A SUGAR CHAIN THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
(MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

SUGAR CHAIN NAME /STRUCTURE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
SUGAR CHAIN A	1002	2	501	15710	55	2
SUGAR CHAIN B	840	2	420	8340	34	3
SUGAR CHAIN C	1280	2	640	10754	42	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A CHEMICAL SUBSTANCE THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
(MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

CHEMICAL SUBSTANCE NAME/STRUCTURE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
CHEMICAL SUBSTANCE A	270	1	270	85510	23	2
CHEMICAL SUBSTANCE B	358	1	358	9840	47	2
CHEMICAL SUBSTANCE C	682	2	341	20764	82	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF AN ION SPECIES DERIVED FROM NOISE OR IMPURITIES
(MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
361	1	361	-	15	-
640	1	640	-	40	-
740	1	740	-	31	-
⋮	⋮	⋮	⋮	⋮	⋮

FIG. 6

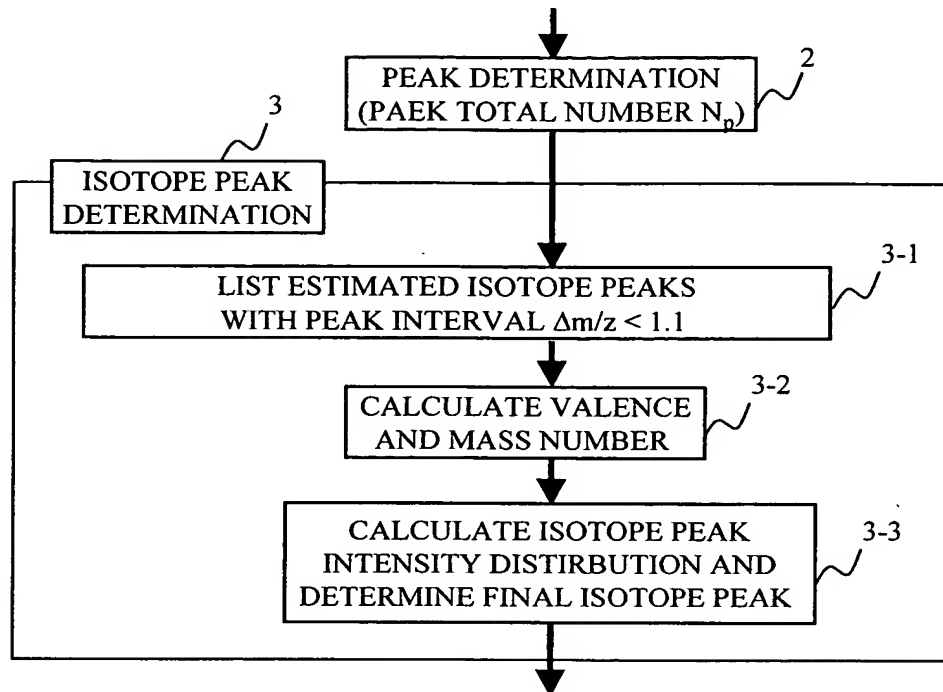


FIG. 7

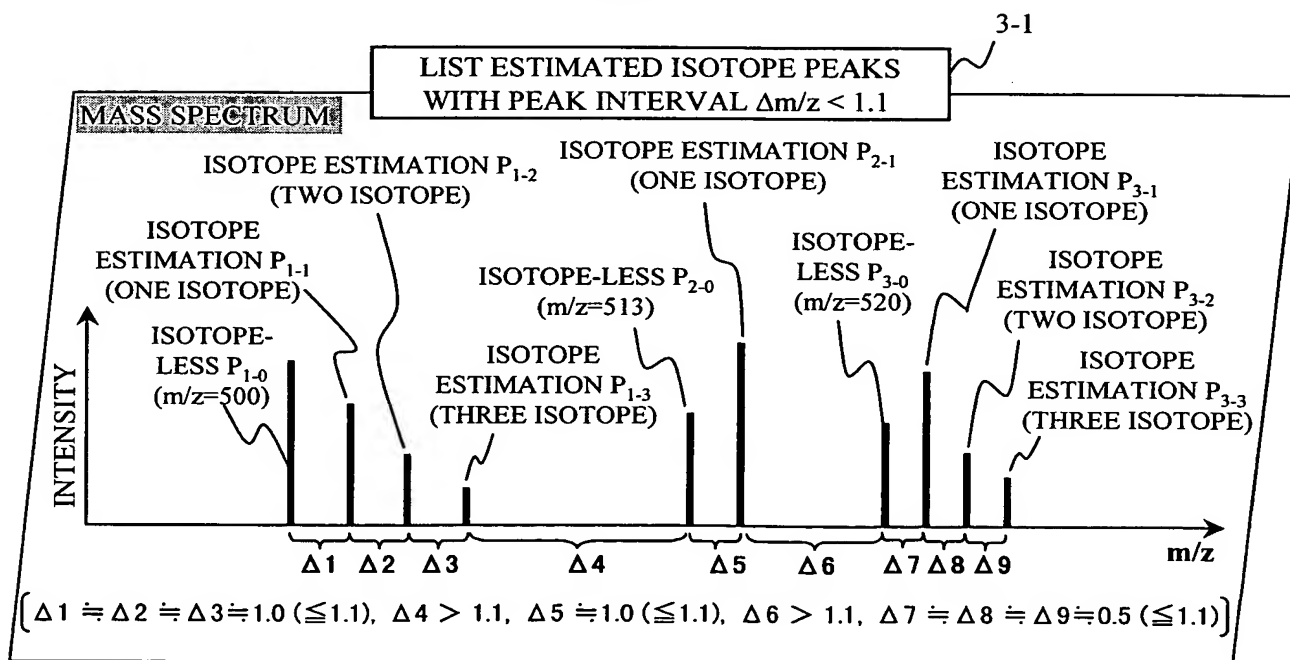


FIG. 8

CALCULATION OF VALENCE AND MASS NUMBER

3-2

 $(m_H : \text{MASS NUMBER OF PROTON})$

ISOTOPE-LESS PEAK P_{1-0}
 PEAK WITH ONE ISOTOPE P_{1-1}
 PEAK WITH TWO ISOTOPE P_{1-2}
 PEAK WITH THREE ISOTOPE P_{1-3}

$> \Delta 1$
 $> \Delta 2$
 $> \Delta 3$



$\Delta 1 \equiv \Delta 2 \equiv \Delta 3 \equiv 1.0 = \Delta(C^{13}-C^{12})/z = 1.0/z \Rightarrow$
 VALENCE $z=1$
 MASS NUMBER m_{p1} OF P_{1-0} IS
 499 FROM $m/z=500=(m_{p1}+m_H \times z)/z$

ISOTOPE-LESS PEAK P_{2-0}
 PEAK WITH ONE ISOTOPE P_{2-1}

$> \Delta 5$



$\Delta 5 \equiv 1.0 = \Delta(C^{13}-C^{12})/z = 1.0/z \Rightarrow$
 VALENCE $z=1$
 MASS NUMBER m_{p2} OF P_{2-0} IS
 512 FROM $m/z=513=(m_{p1}+m_H \times z)/z$

ISOTOPE-LESS PEAK P_{3-0}
 PEAK WITH ONE ISOTOPE P_{3-1}
 PEAK WITH TWO ISOTOPE P_{3-2}
 PEAK WITH THREE ISOTOPE P_{3-3}

$> \Delta 7$
 $> \Delta 8$
 $> \Delta 9$



$\Delta 7 \equiv \Delta 8 \equiv \Delta 9 \equiv 0.5 = \Delta(C^{13}-C^{12})/z = 1.0/z \Rightarrow$
 VALENCE $z=2$
 MASS NUMBER m_{p3} OF P_{3-0} IS
 1038 FROM $m/z=520=(m_{p3}+m_H \times z)/z$

FIG. 9 A

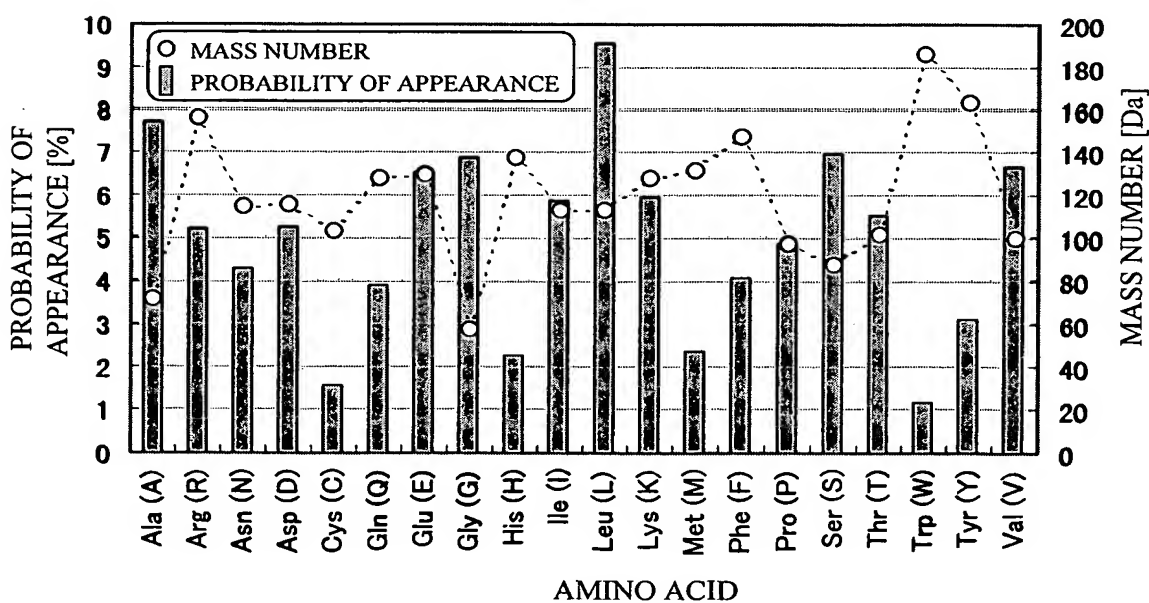


FIG. 9 B

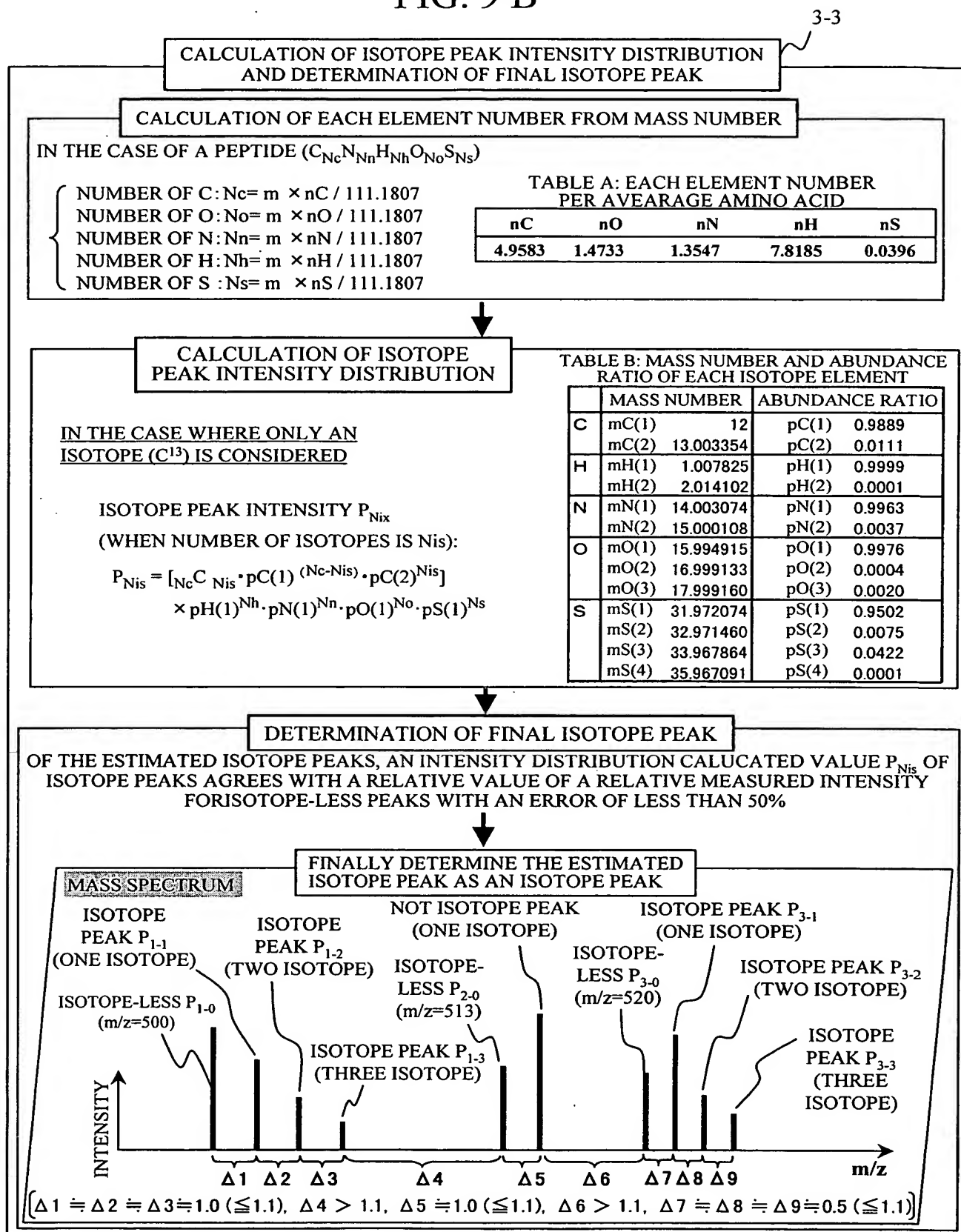


FIG. 10

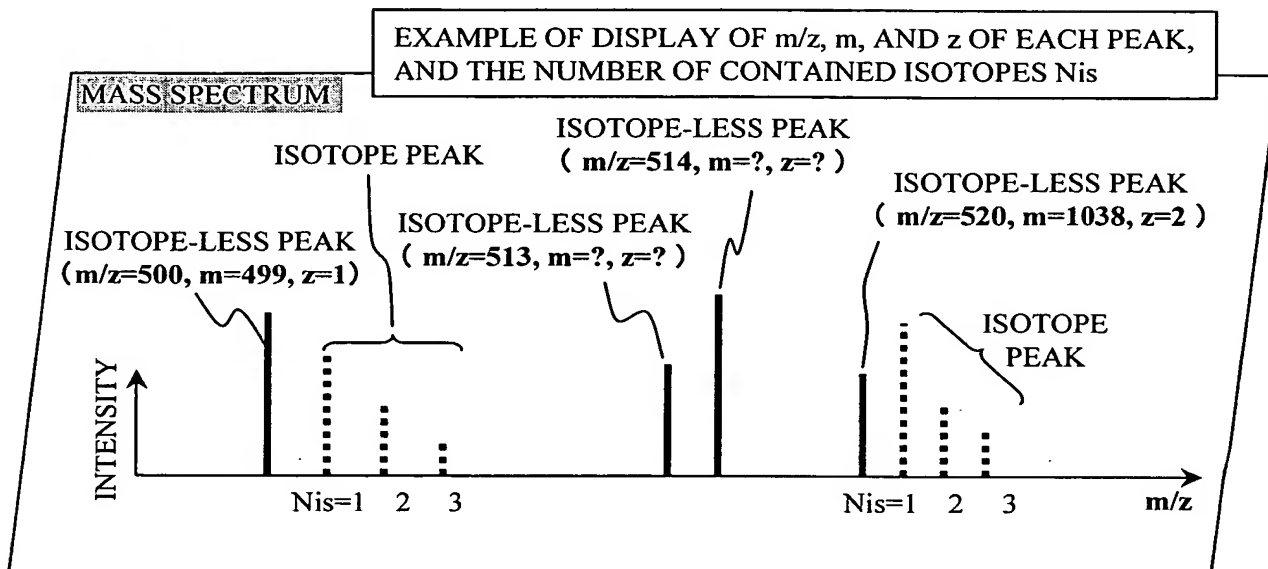


FIG. 11

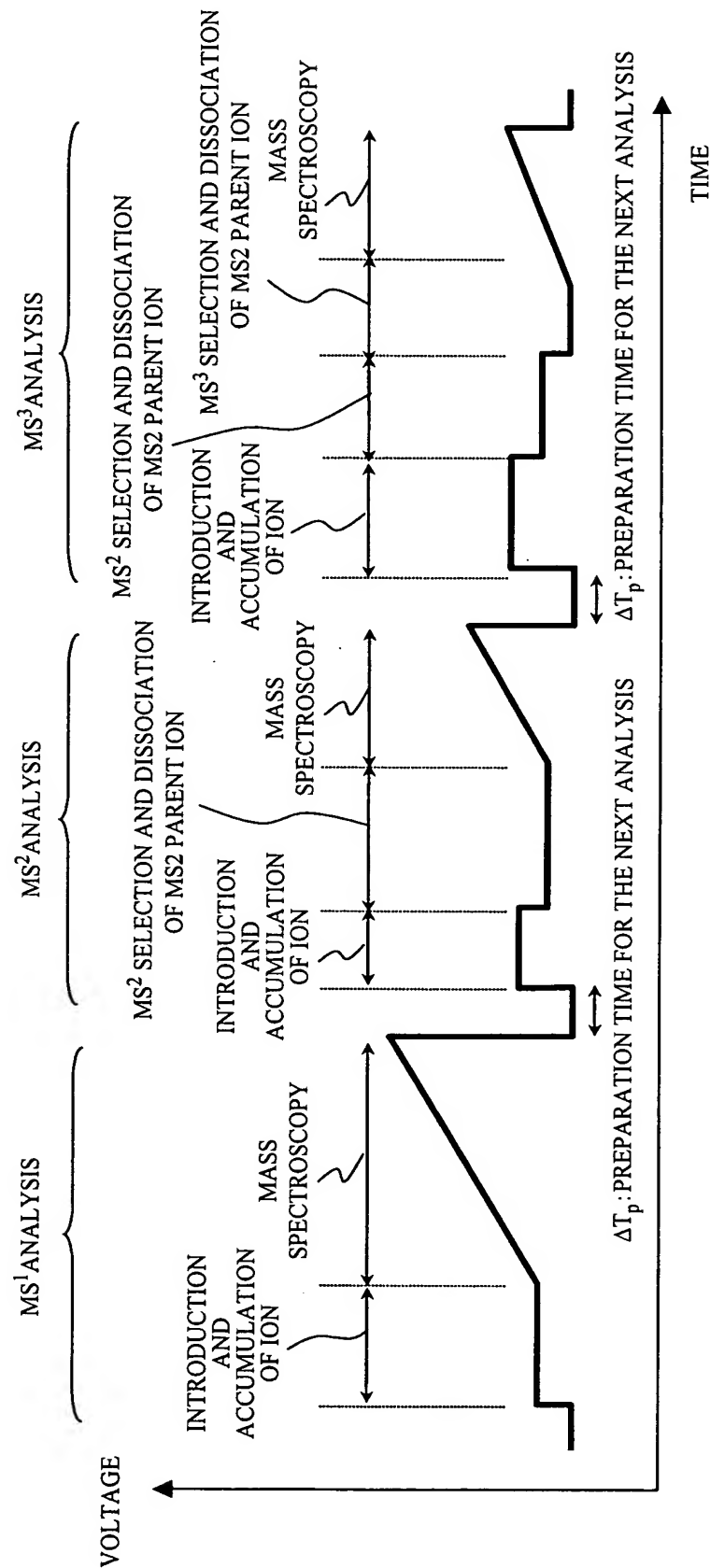


FIG. 12

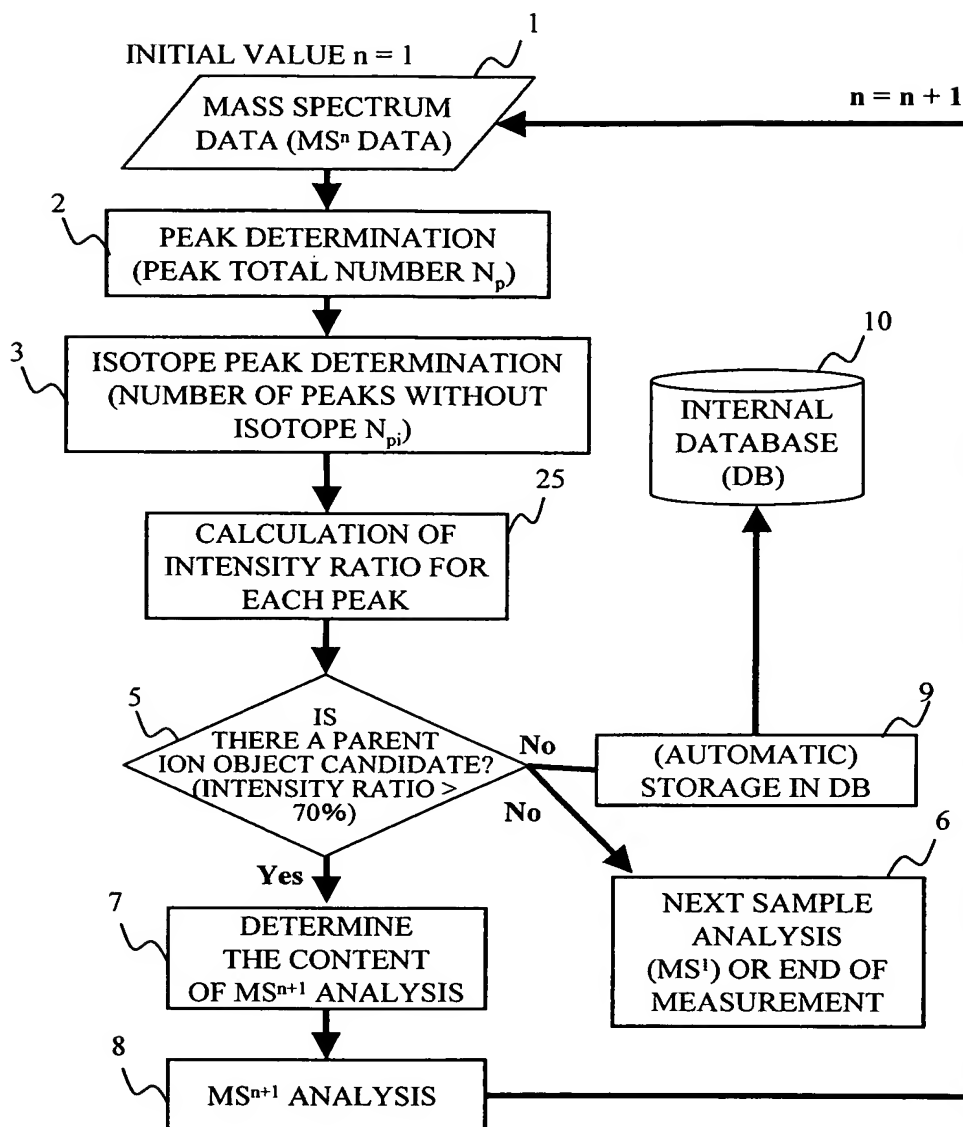


FIG. 13

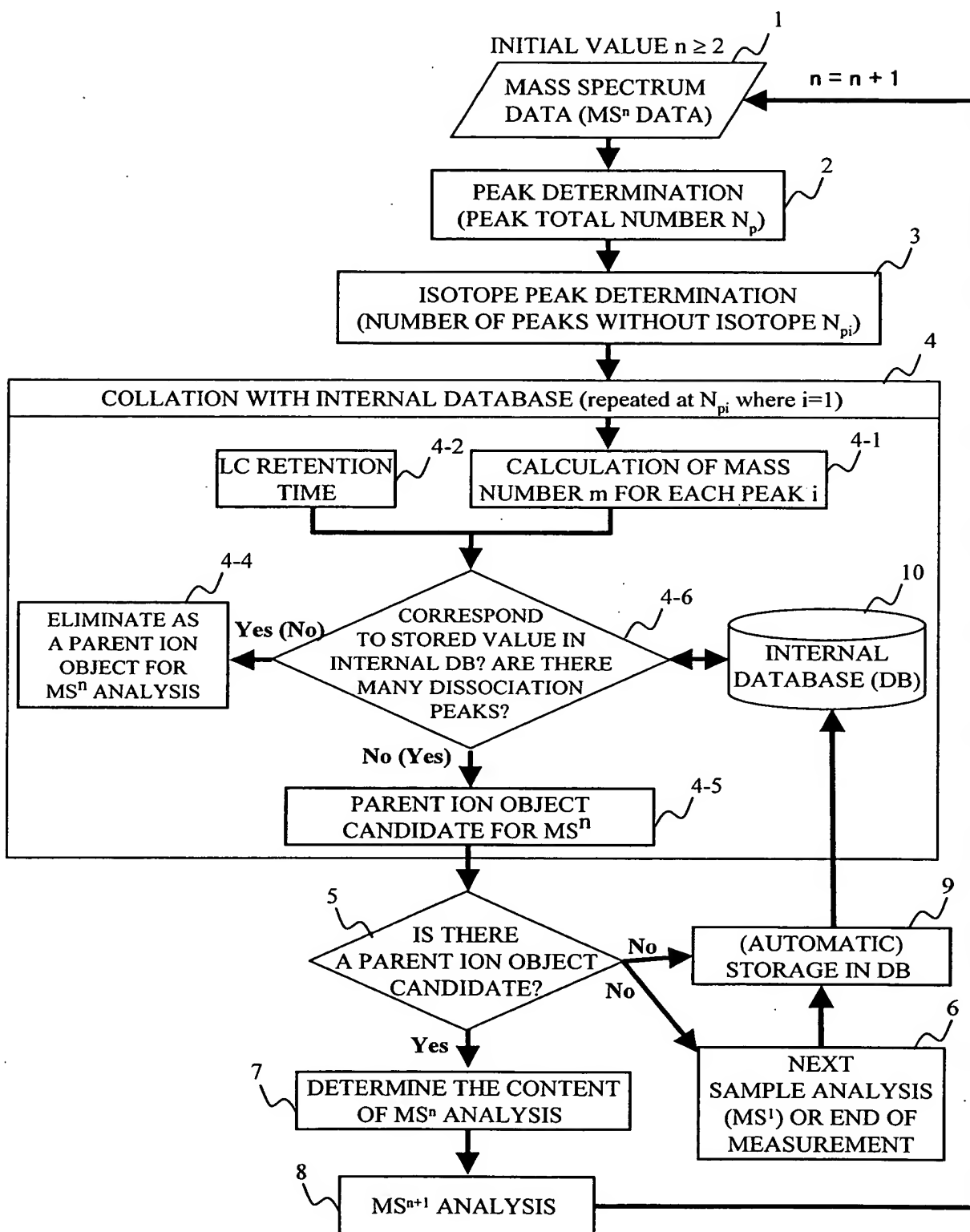


FIG. 14

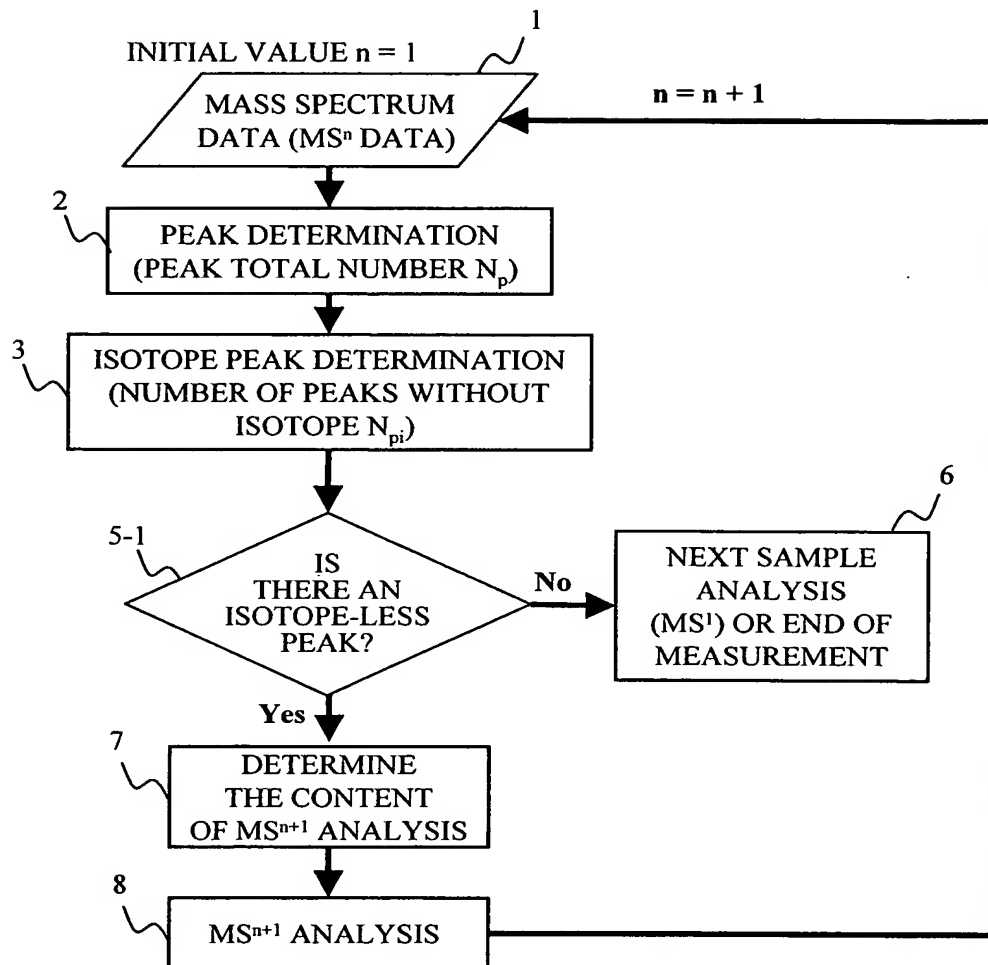


FIG. 15

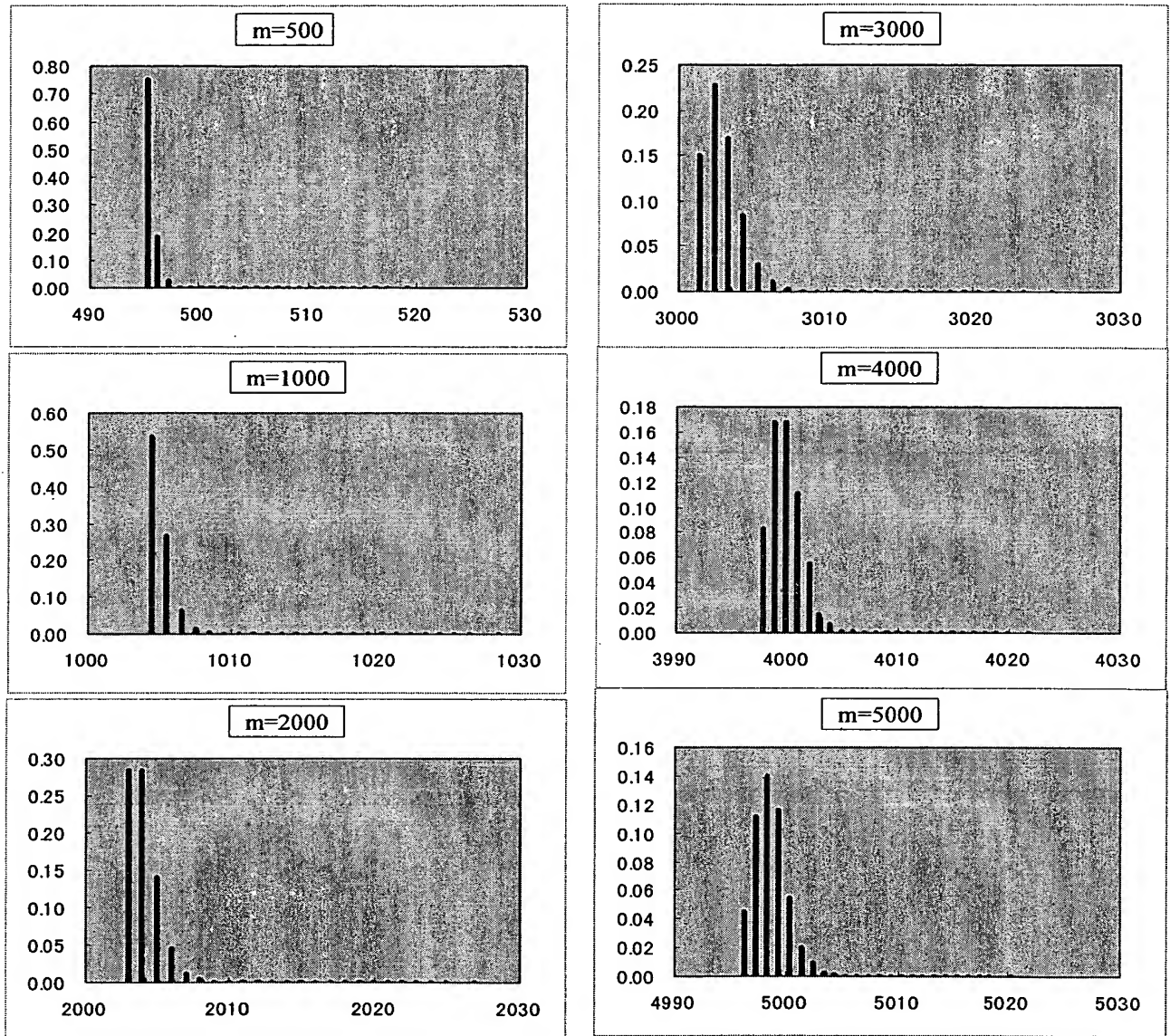
ISOTOPE PEAK INTENSITY DISTRIBUTION
PATTERNS DEPENDING ON ION MASS NUMBER

FIG. 16

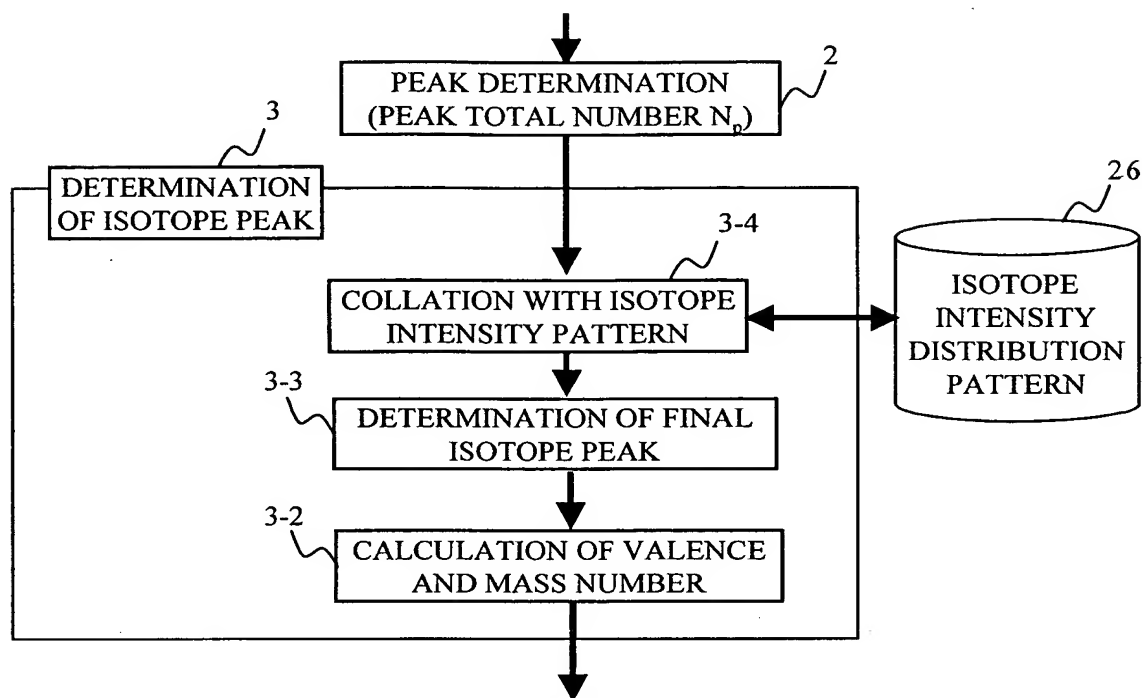


FIG. 17

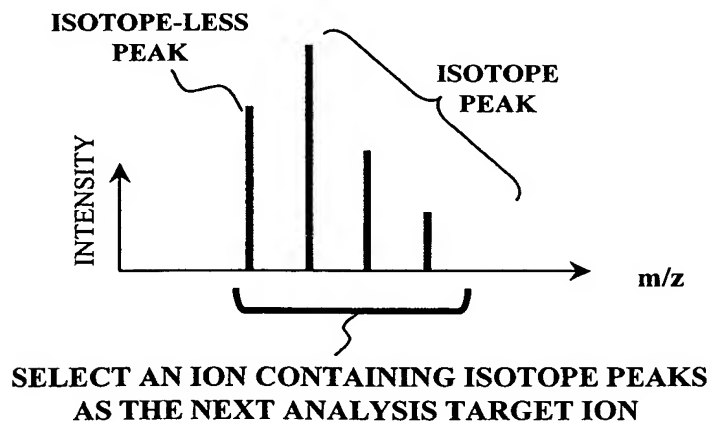


FIG. 18

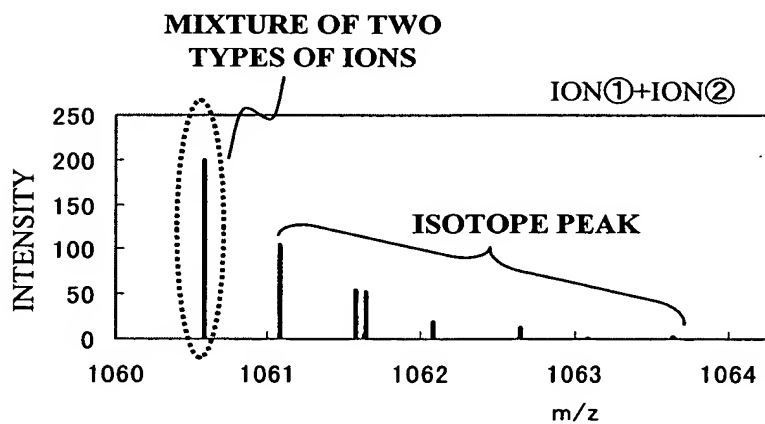
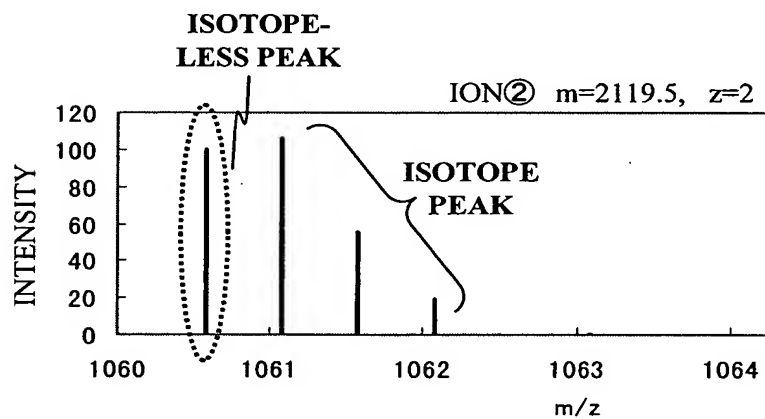
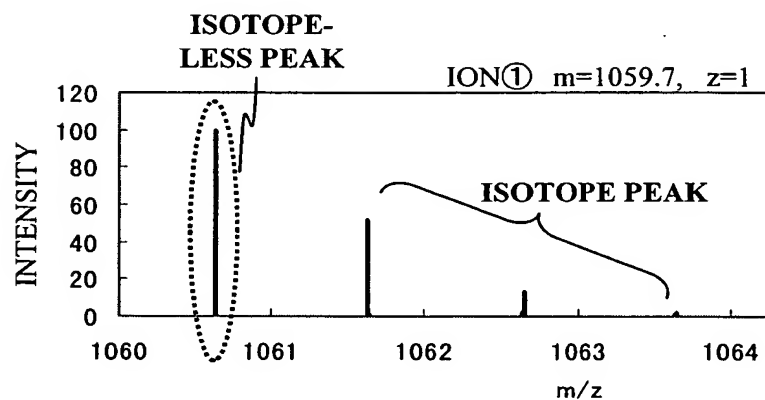


FIG. 19

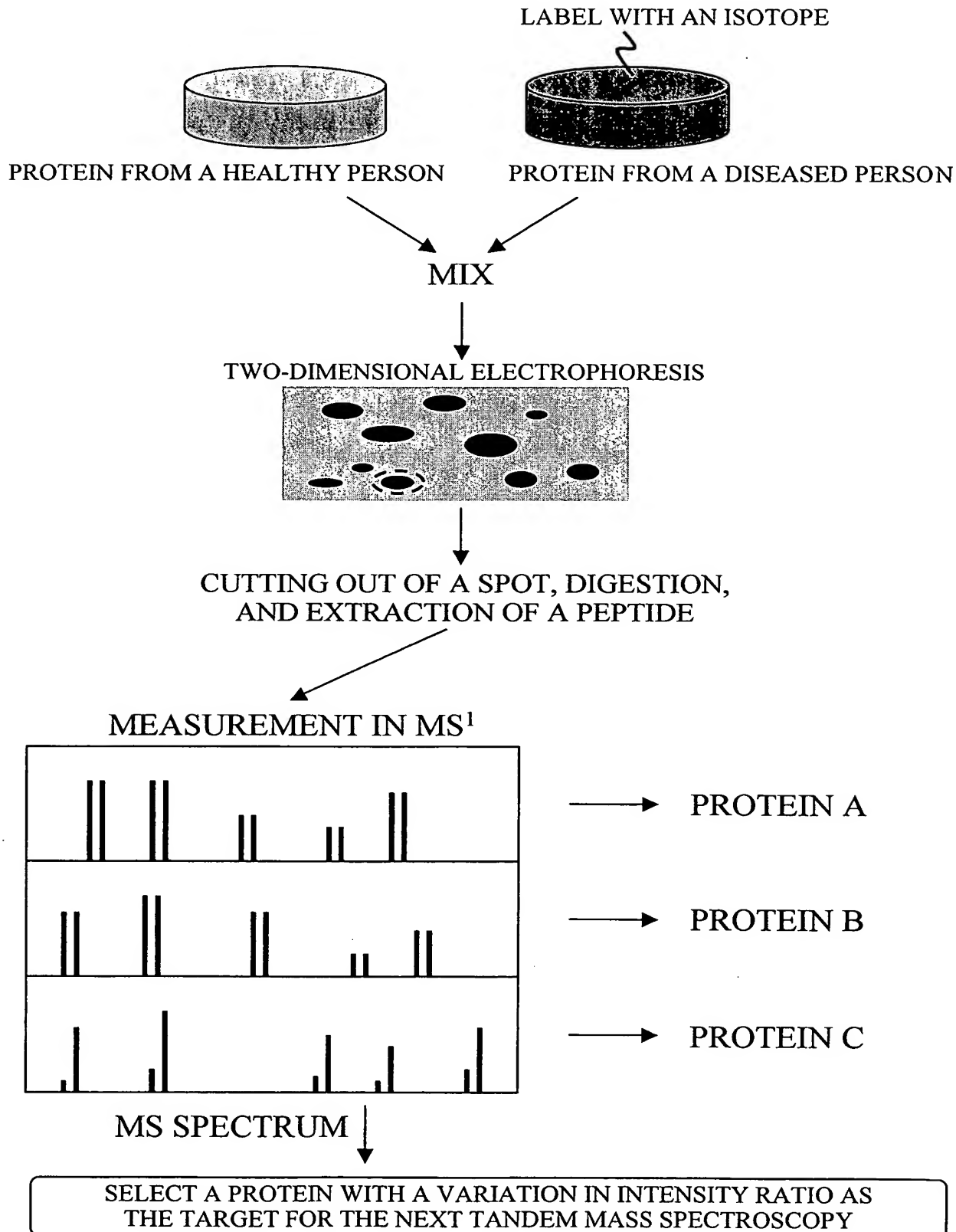


FIG. 20

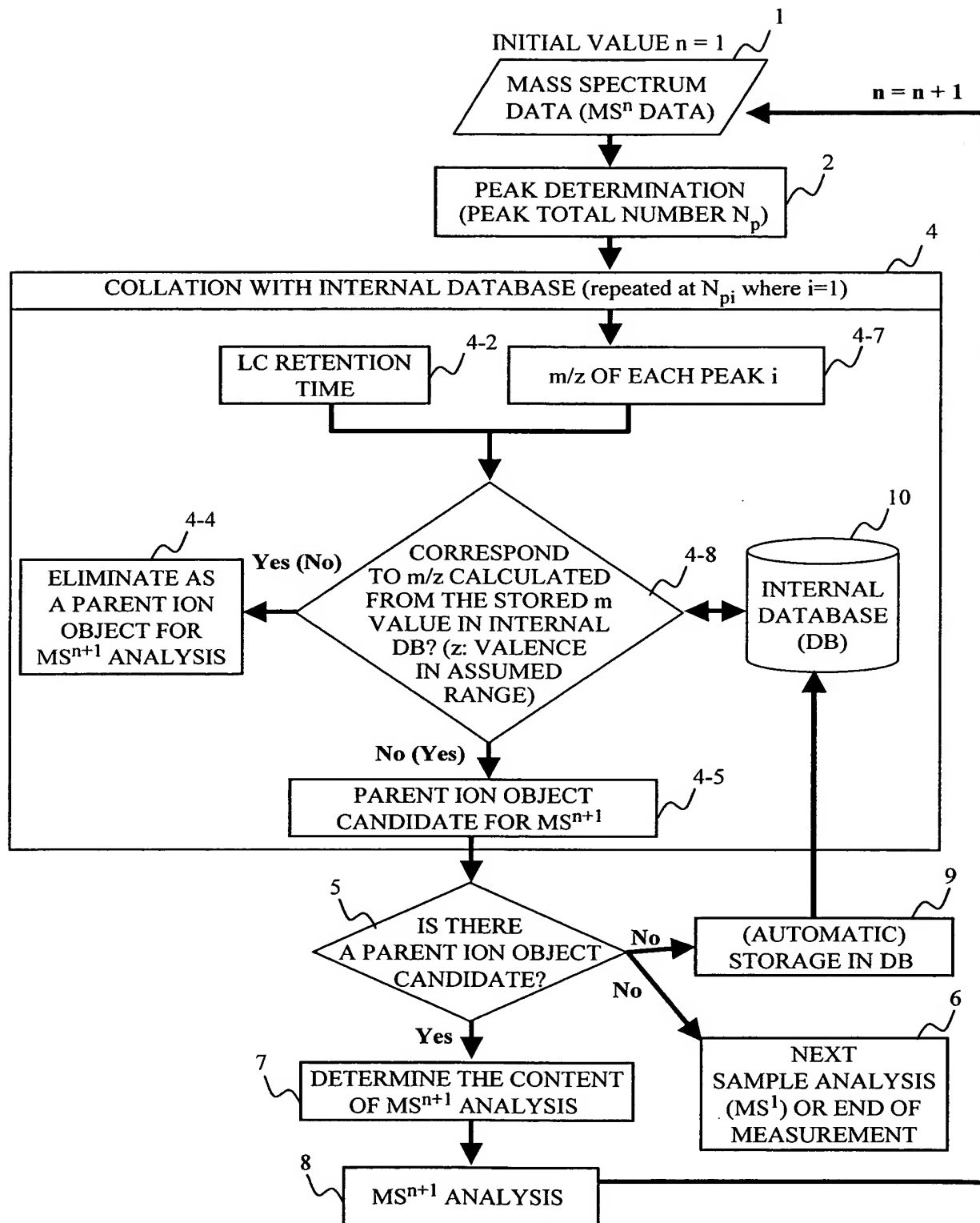


FIG. 21

MASS SPECTRUM

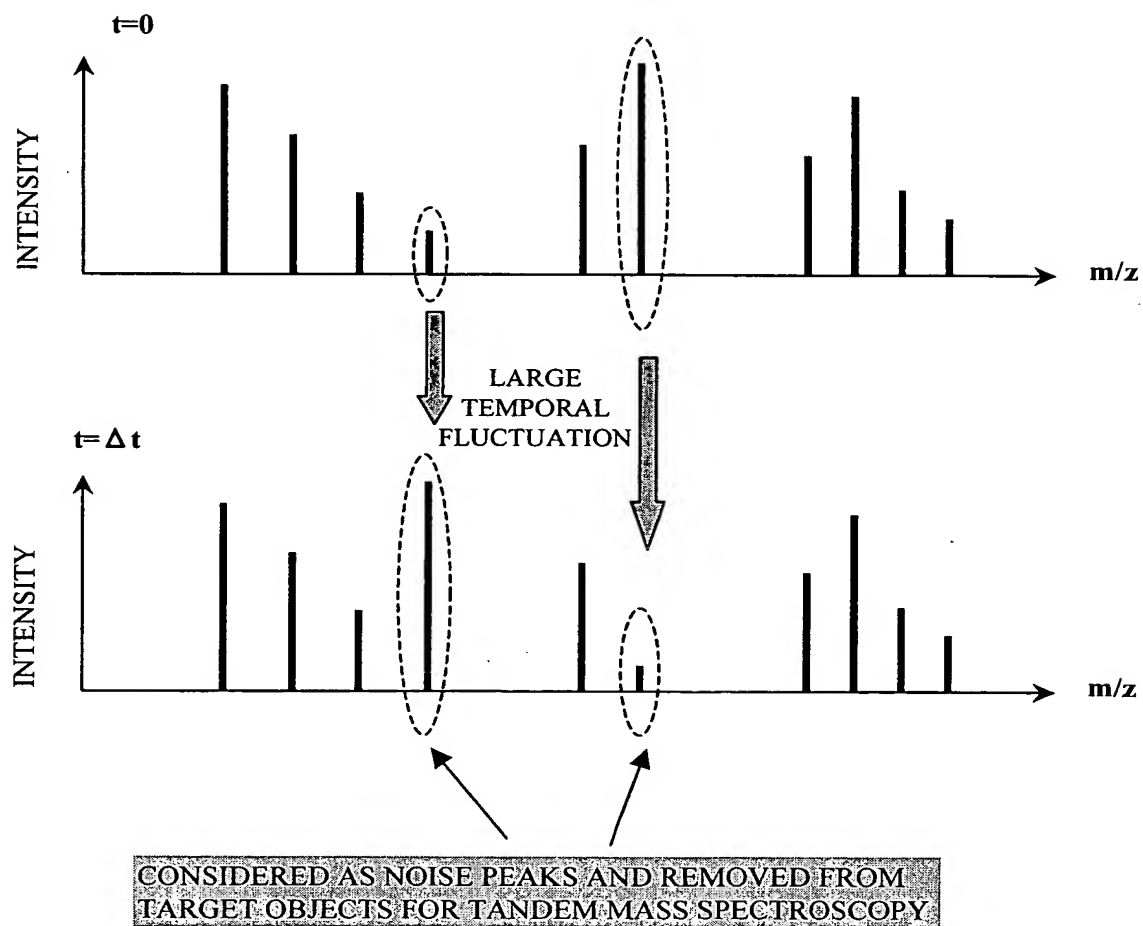


FIG. 22 a

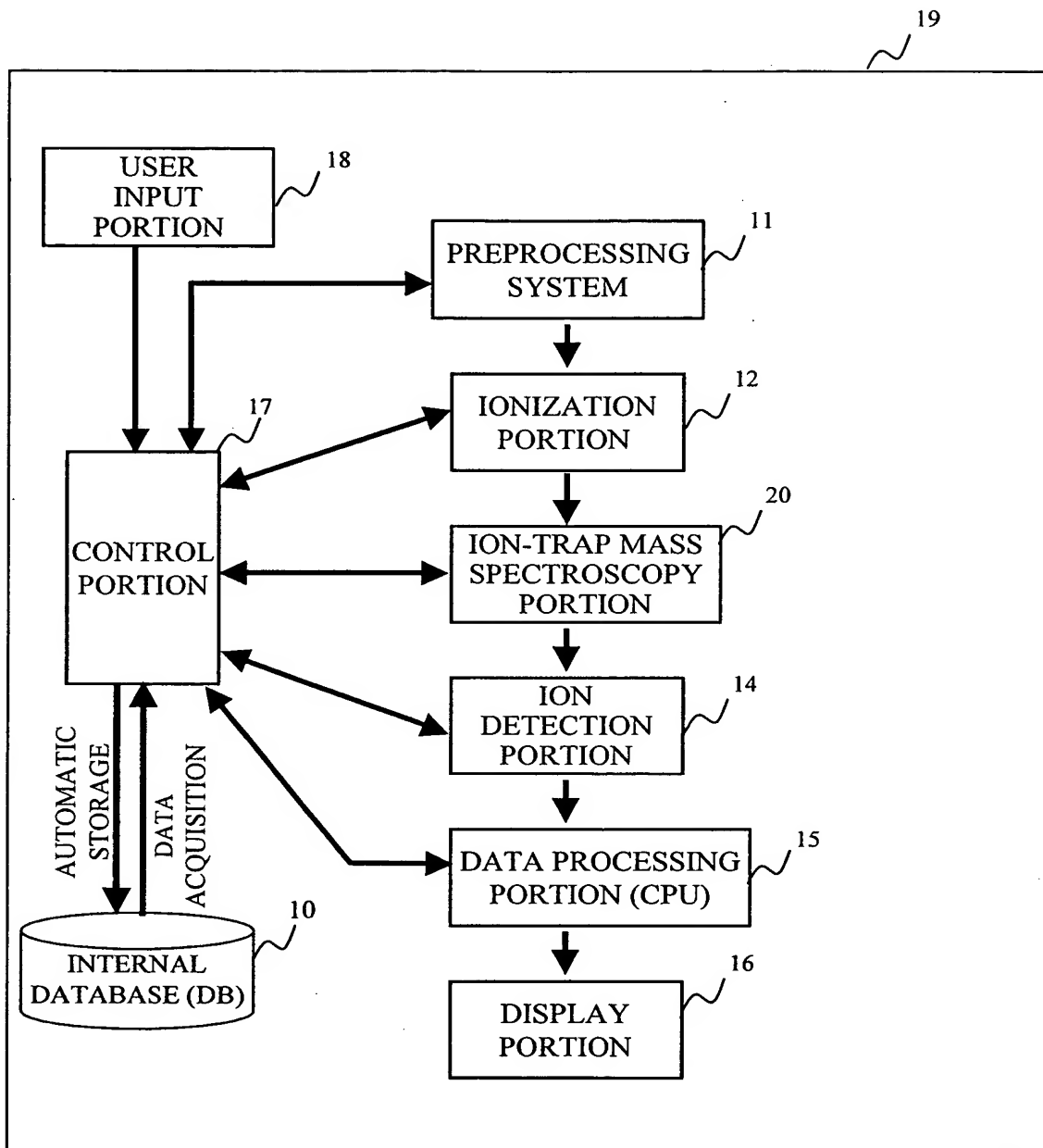


FIG. 22 b

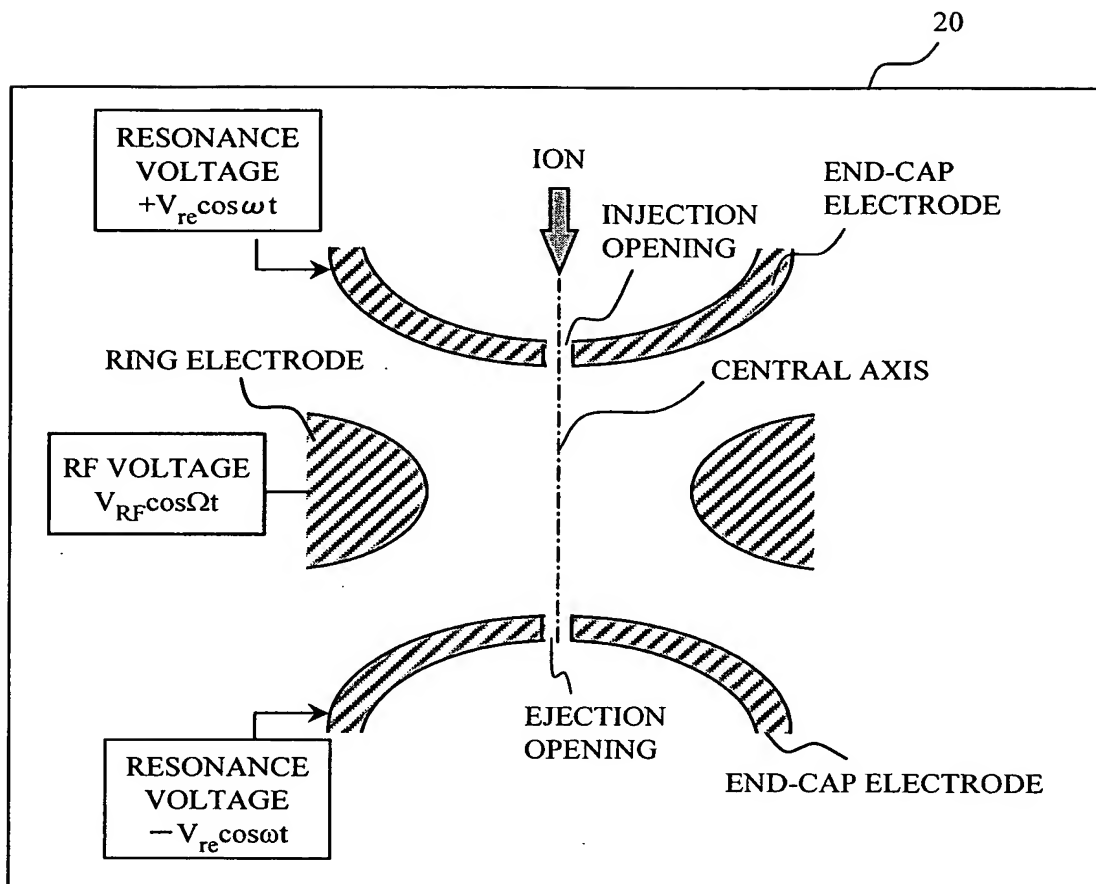


FIG. 23

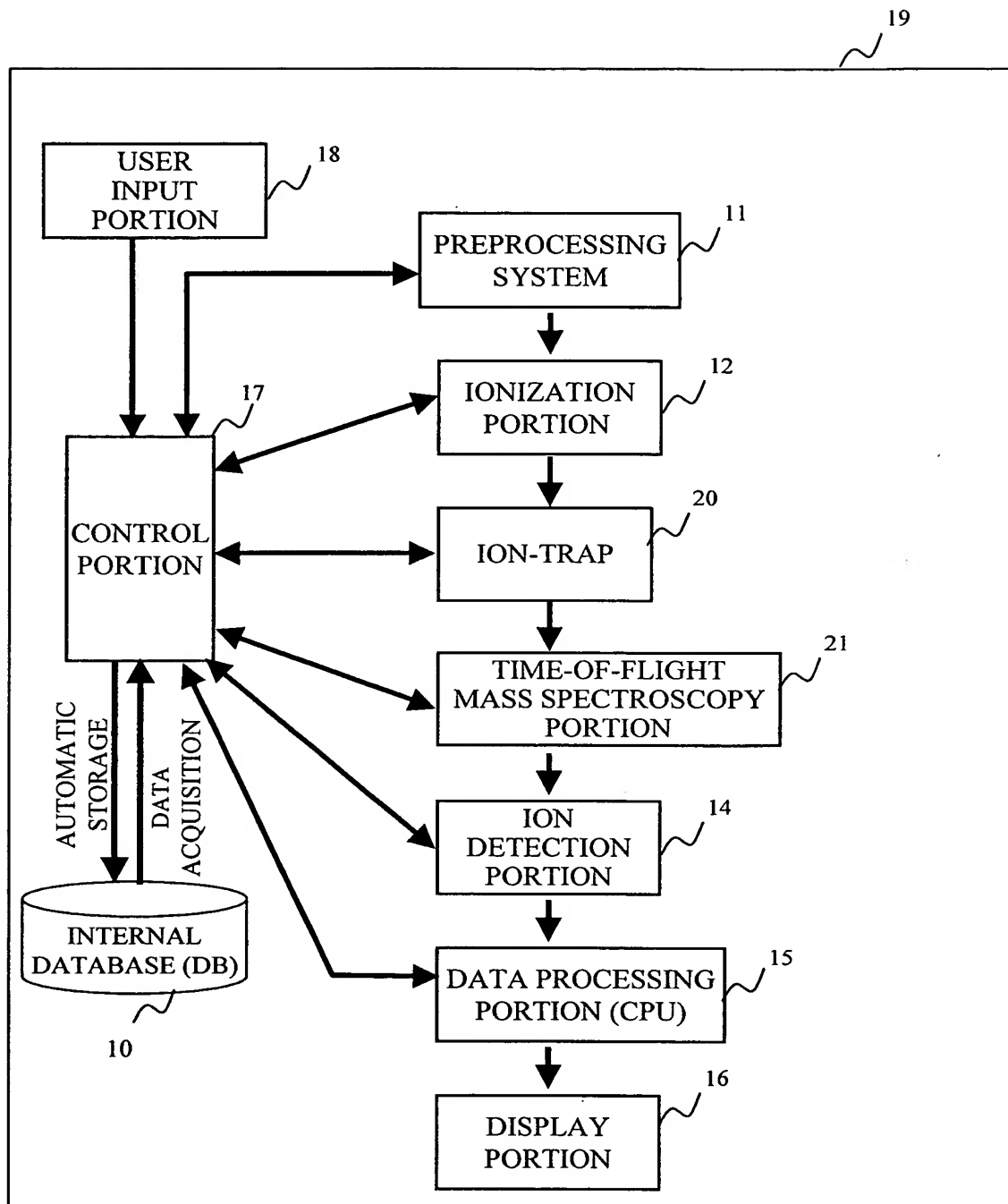


FIG. 24 a

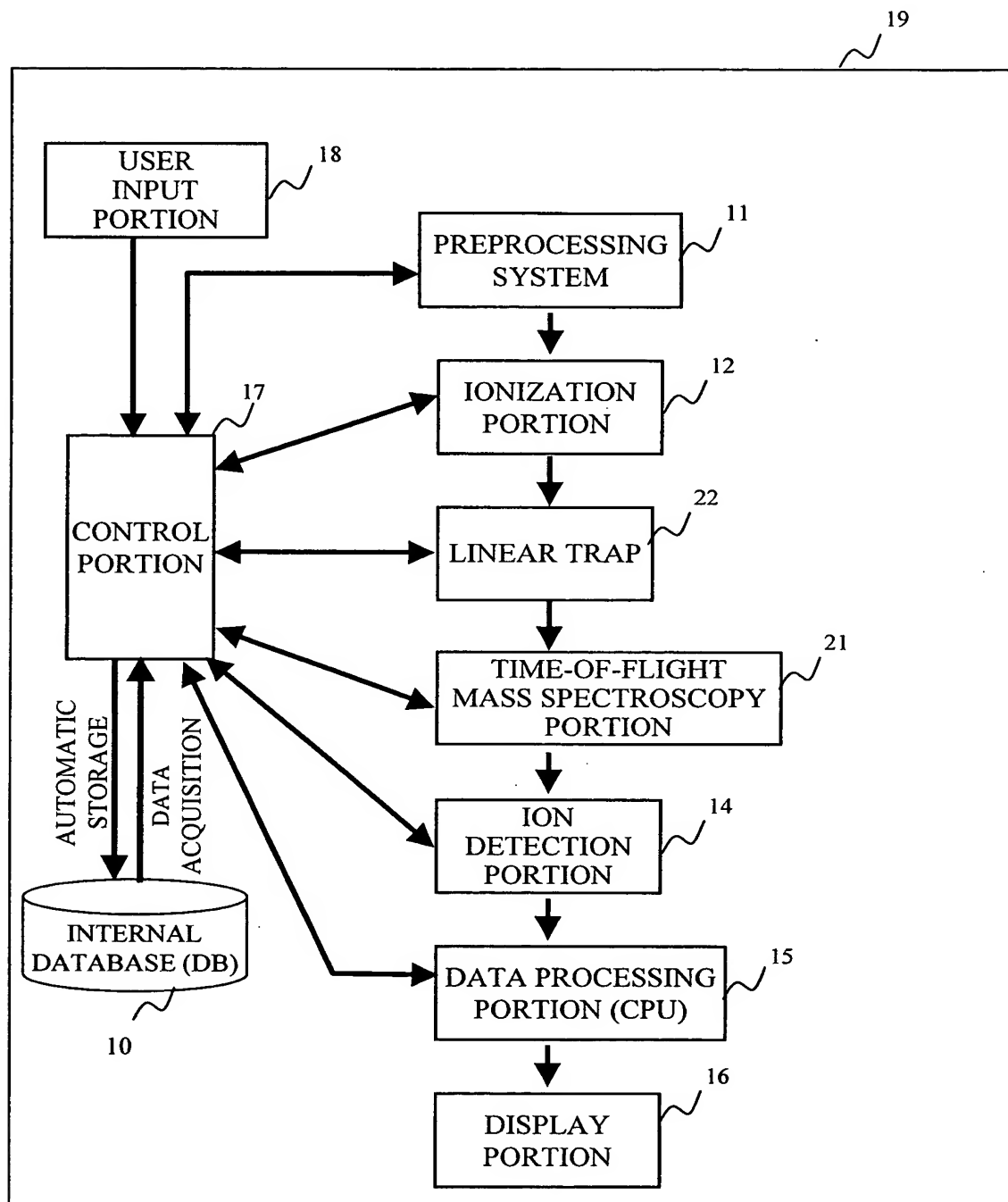


FIG. 24 b

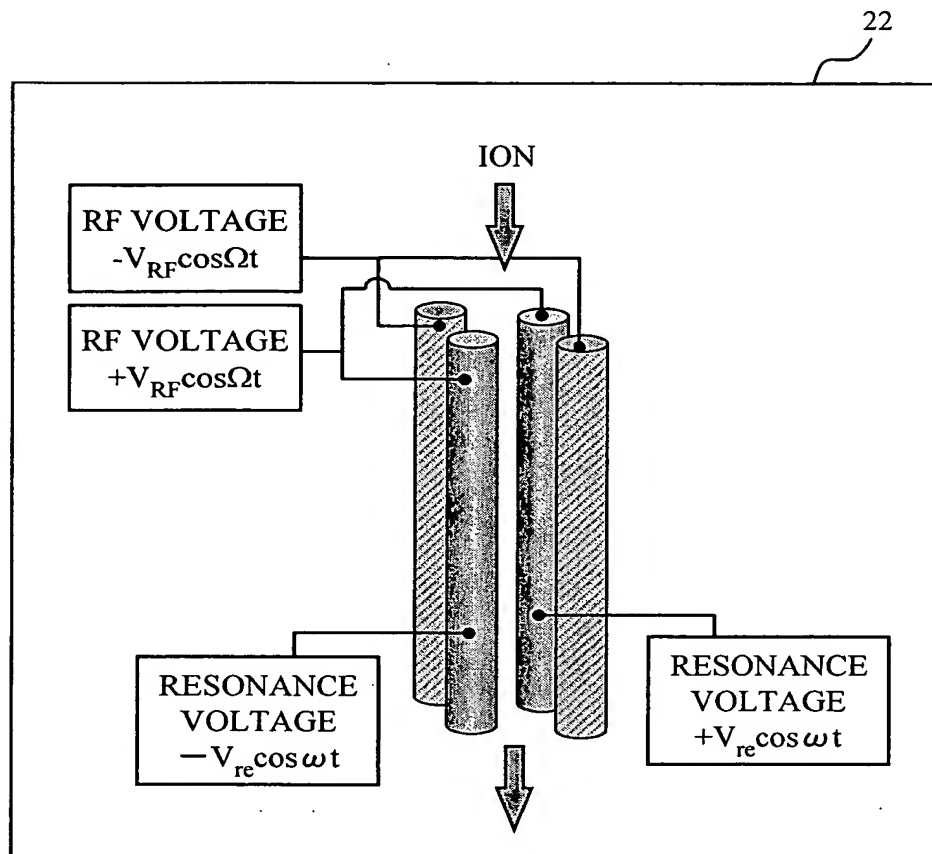


FIG. 25

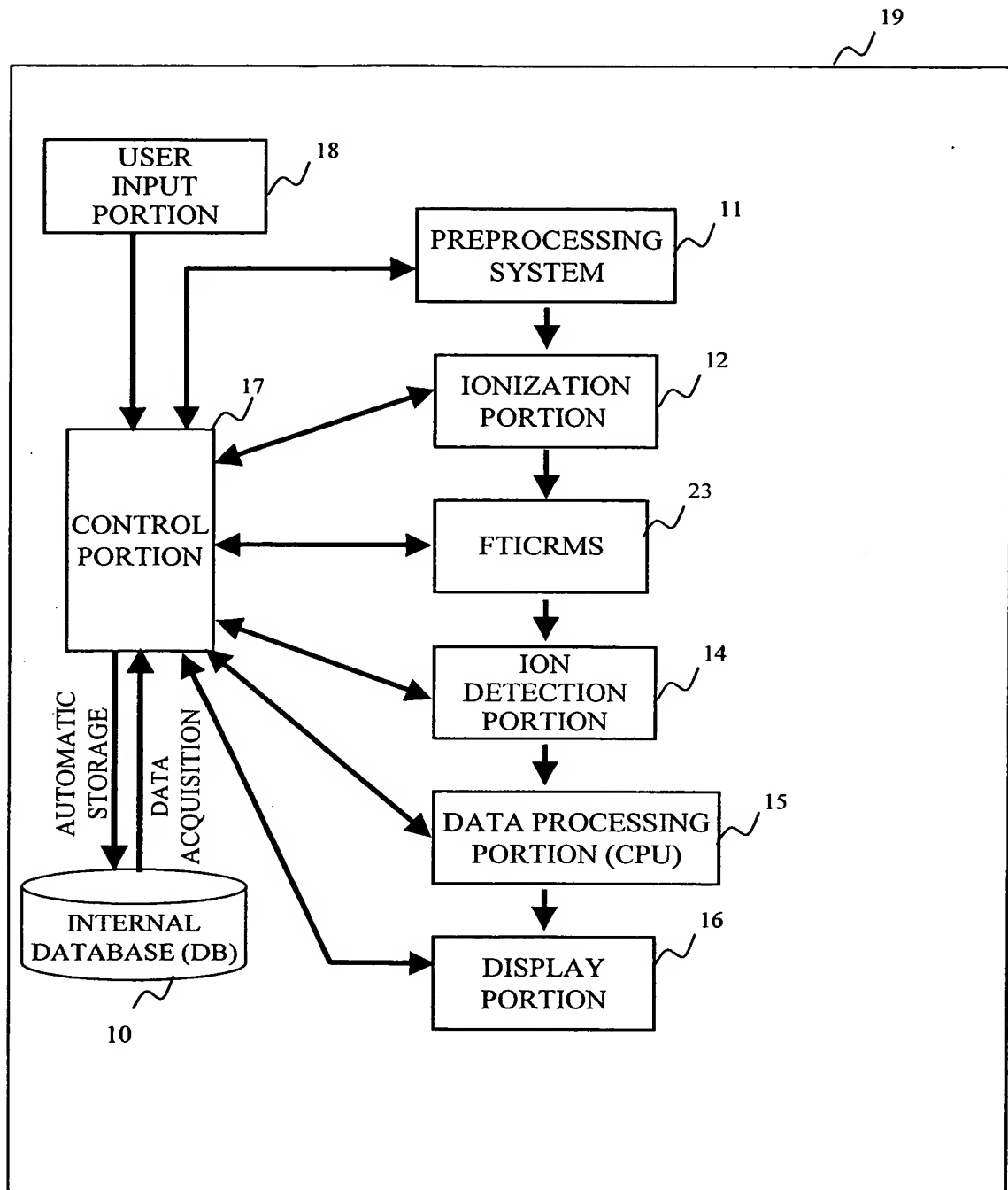


FIG. 26

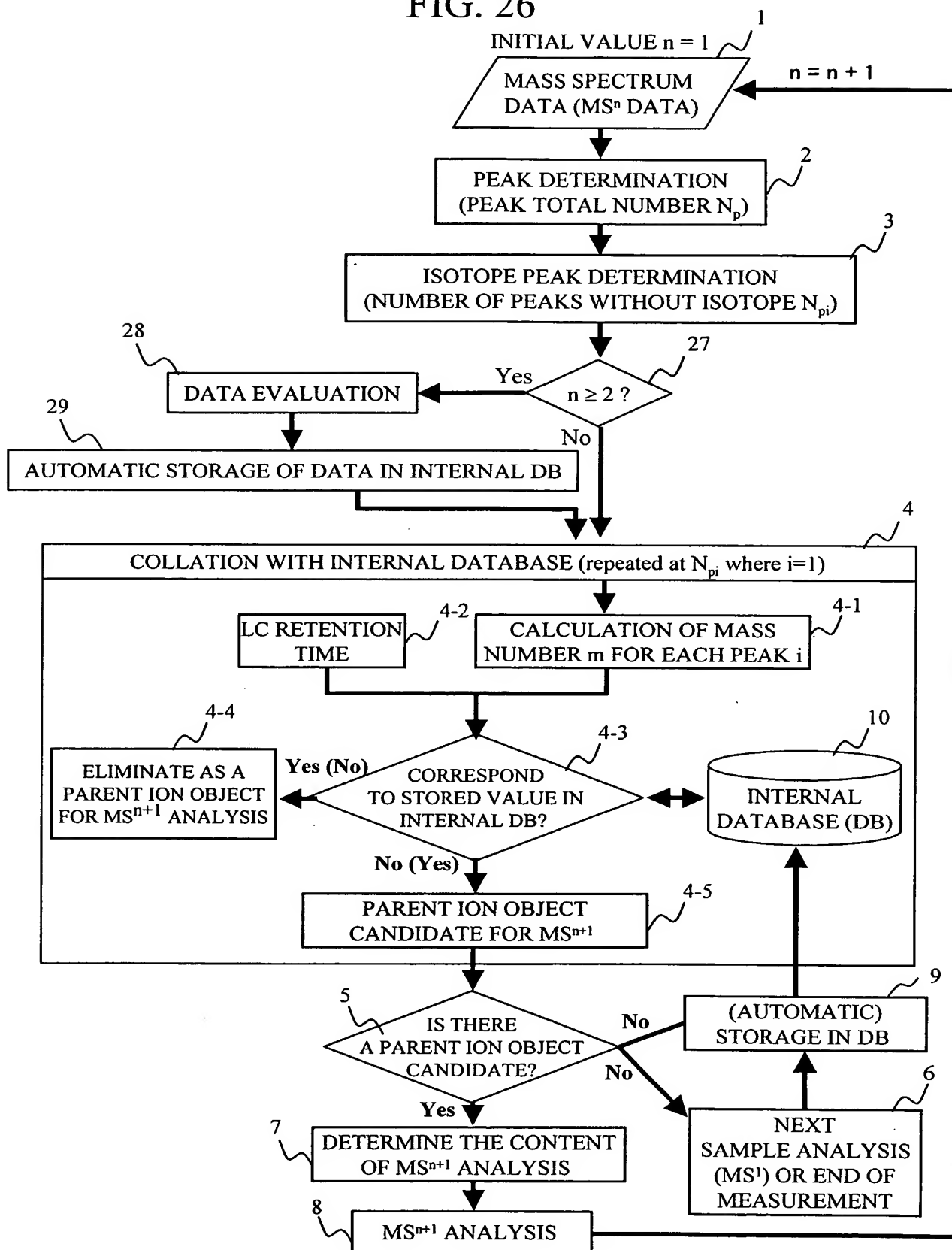


FIG. 27

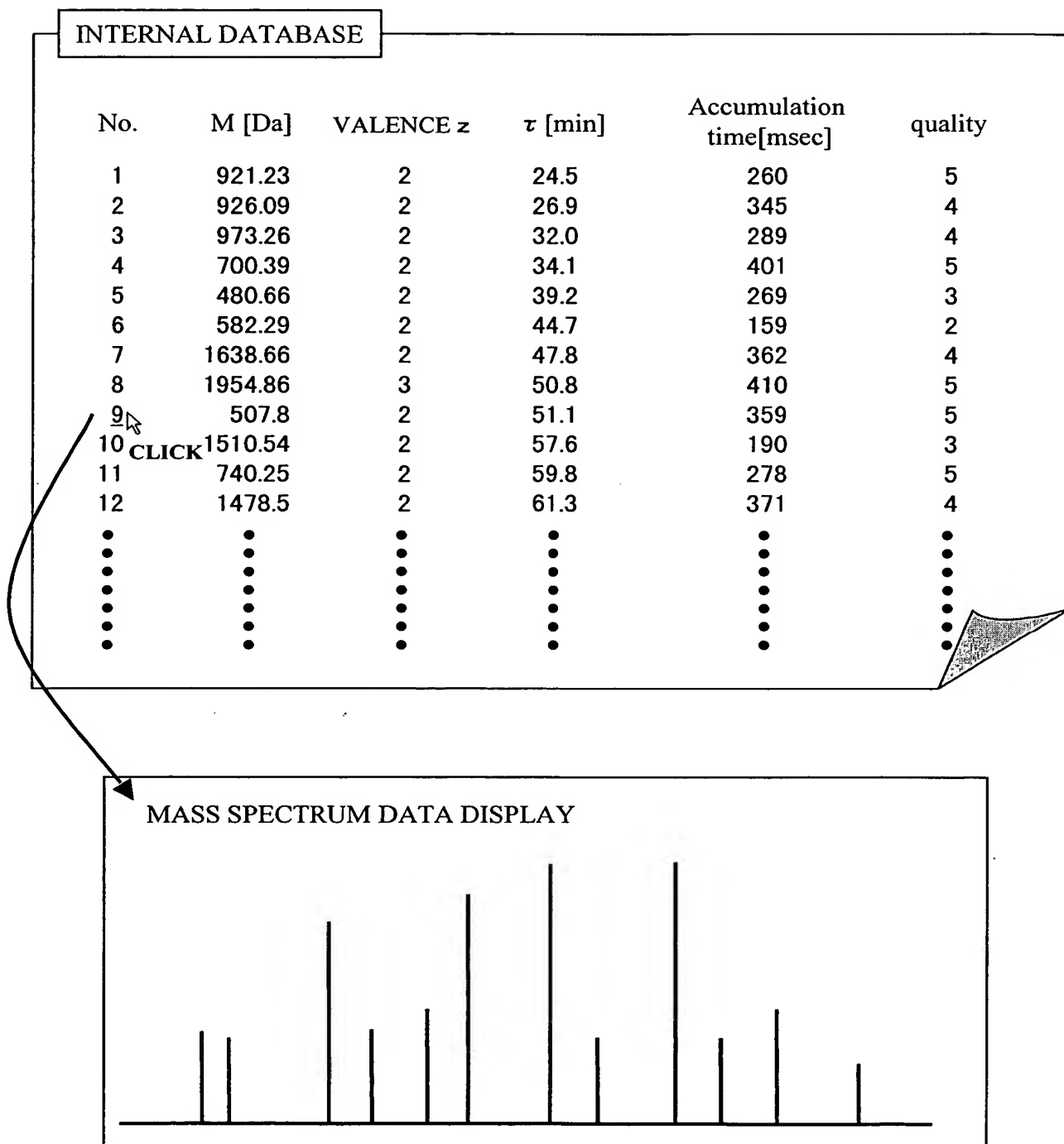


FIG. 28 A

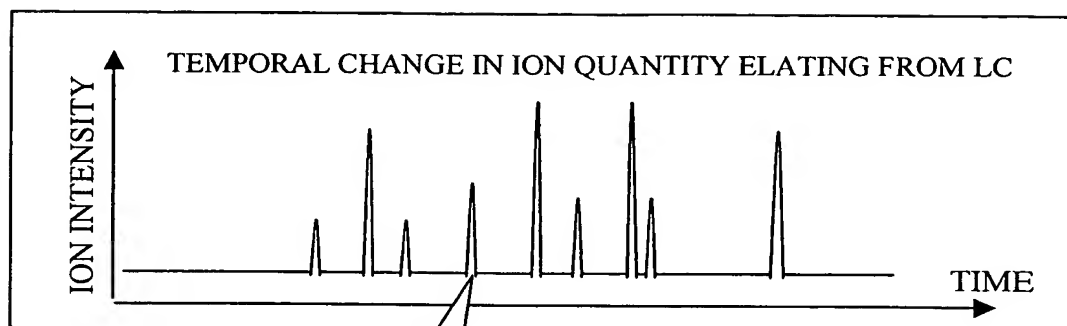


FIG. 28 B

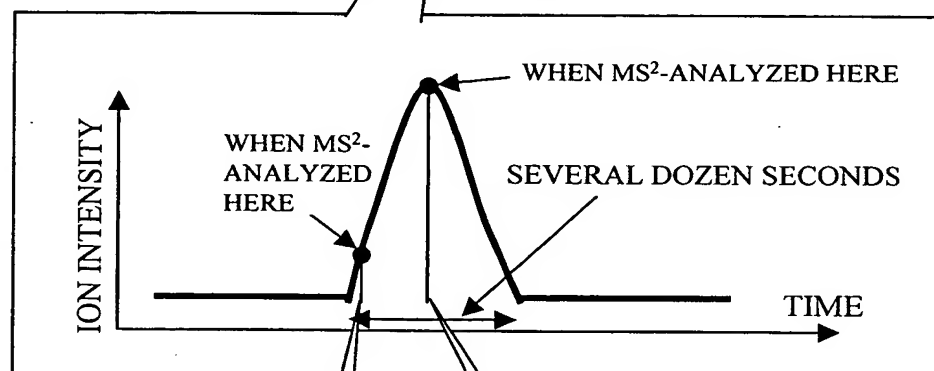


FIG. 28 C

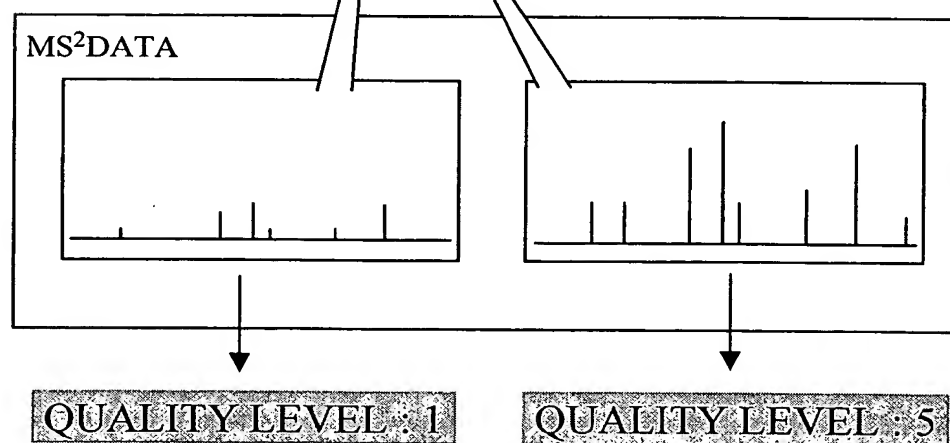


FIG. 29

INTERNAL DATABASE					
No.	M [Da]	VALENCE z	τ [min]	Accumulation time[msec]	quality
1	921.23	2	24.5	260	5
2	926.09	2	26.9	345	4
3	973.26	2	32.0	289	4
4	700.39	2	34.1	401	5
5	480.66	2	39.2	269	3
6	582.29	2	42.7	159	2
7	<u>1638.66</u>	<u>2</u>	<u>47.6</u>	362	2
8	<u>1638.67</u>	<u>2</u>	<u>47.7</u>	359	2
9	<u>1638.65</u>	<u>2</u>	<u>47.7</u>	339	3
10	<u>1638.66</u>	<u>2</u>	<u>47.7</u>	352	3
11	<u>1638.67</u>	<u>2</u>	<u>47.8</u>	254	4
12	<u>1638.68</u>	<u>2</u>	<u>47.8</u>	262	5
13	<u>1638.66</u>	<u>2</u>	<u>47.8</u>	219	5
14	<u>1638.65</u>	<u>2</u>	<u>47.8</u>	285	4
15	<u>1638.66</u>	<u>2</u>	<u>47.8</u>	248	5
16	<u>1638.65</u>	<u>2</u>	<u>47.8</u>	299	4
17	<u>1638.68</u>	<u>2</u>	<u>47.9</u>	280	4
18	<u>1638.67</u>	<u>2</u>	<u>47.9</u>	310	3
19	<u>1638.67</u>	<u>2</u>	<u>48.0</u>	307	3
20	<u>1638.64</u>	<u>2</u>	<u>48.0</u>	336	3
21	<u>1638.65</u>	<u>2</u>	<u>48.0</u>	318	3
22	1954.86	3	50.8	410	5
23	507.8	2	51.1	359	5
24	1510.54	2	57.6	190	3
25	740.25	2	59.8	278	5
26	1478.5	2	61.3	371	4
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

CAN BE CONSIDERED AS IDENTICAL ION (BASED ON MASS NUMBER, VALENCE, AND RETENTION TIME)

↓

DELETE REDUNDANT DATA FROM DB

FIG. 30

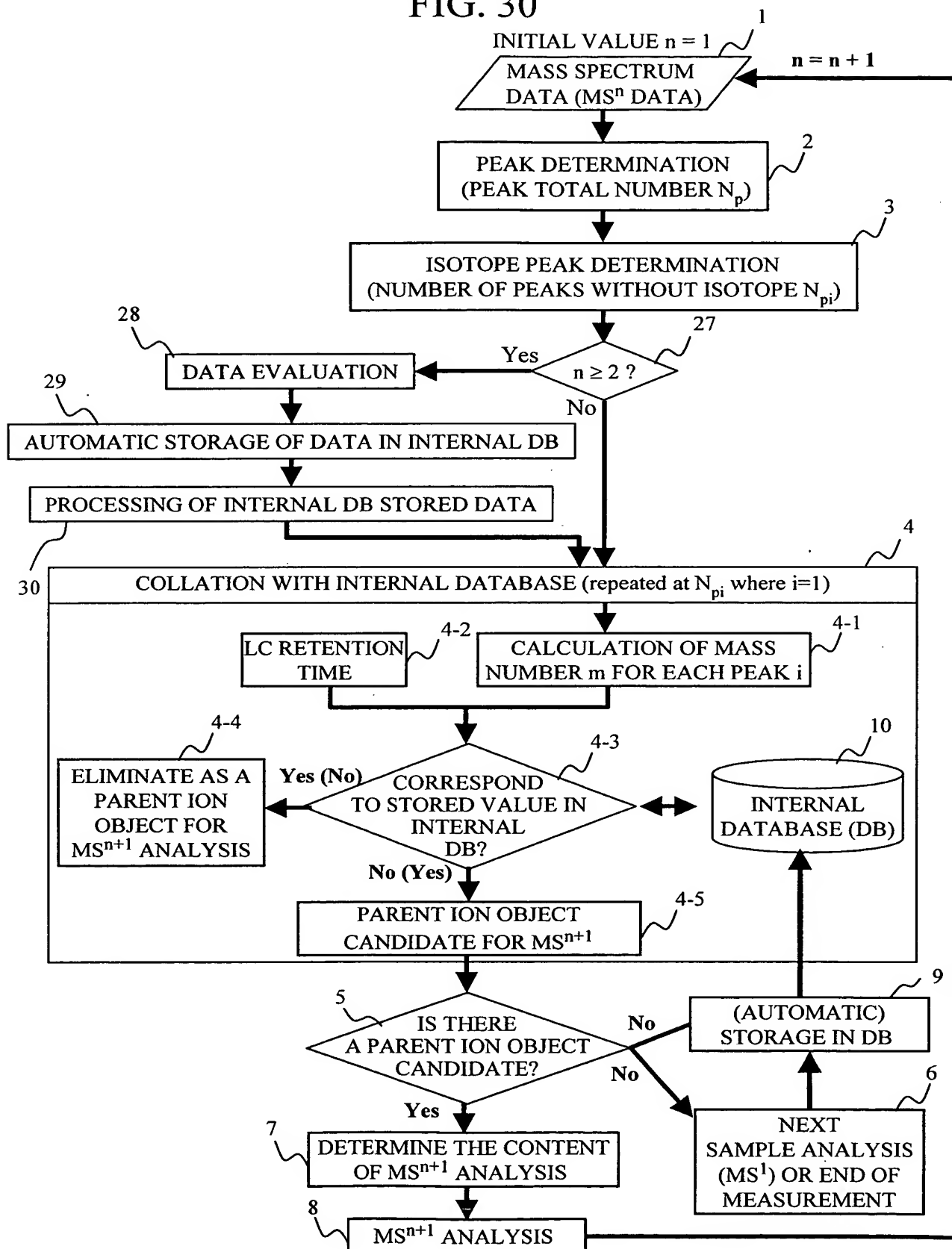


FIG. 31

INTERNAL DATABASE					
No.	M [Da]	VALENCE z	τ [min]	Accumulation time[msec]	quality
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
N	1638.67	2	47.7	359	3
N+1	838.68	1	47.7	439	2
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

MS² ANALYSIS
MS³ ANALYSIS

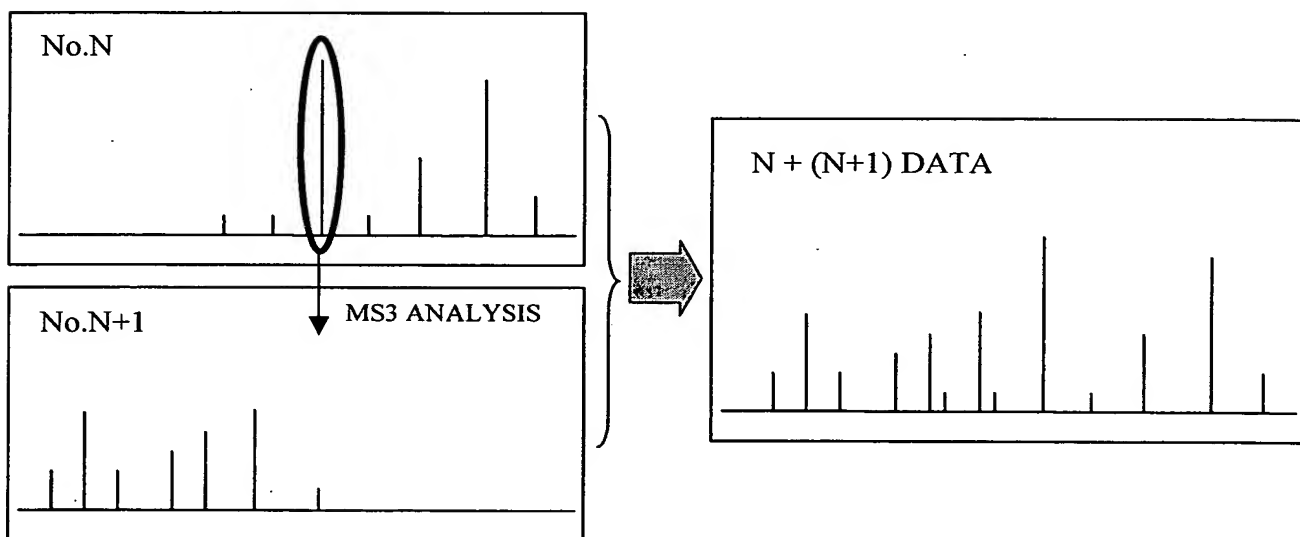


FIG. 32

INTERNAL DATABASE					
No.	M [Da]	VALENCE z	τ [min]	Accumulation time[msec]	quality
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
K	1638.67	2	47.7	359	3
K+1	1638.68	2	47.7	339	3
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

DATA DUE TO COLLISION INDUCED DISSOCIATION (CID)

DATA DUE TO ELECTRON CAPTURE DISSOCIATION (ECD)

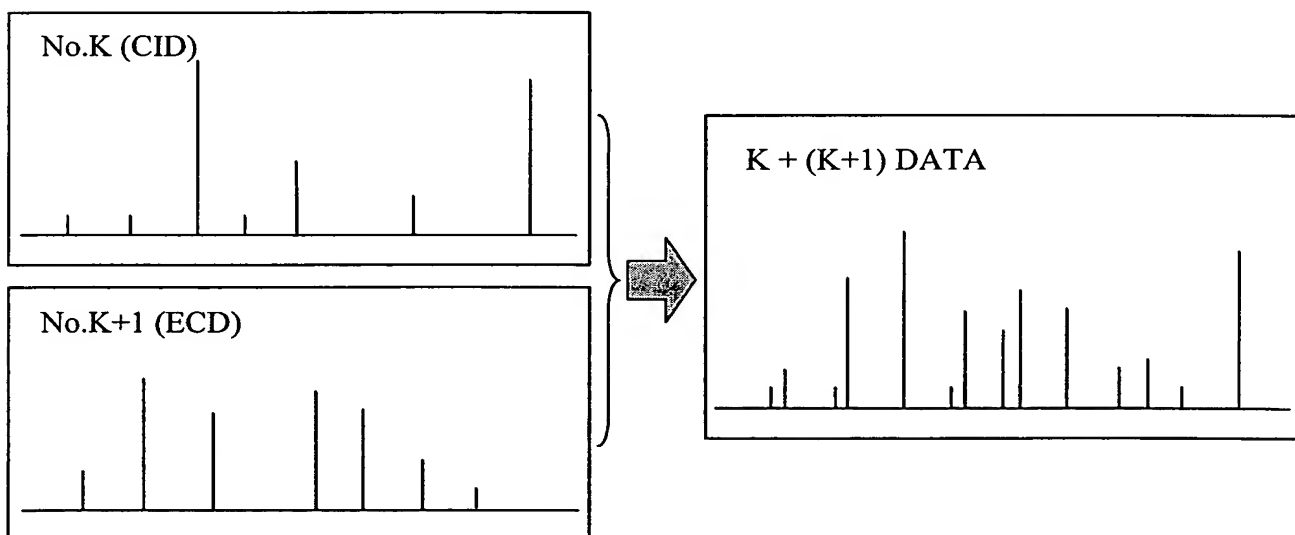


FIG. 33

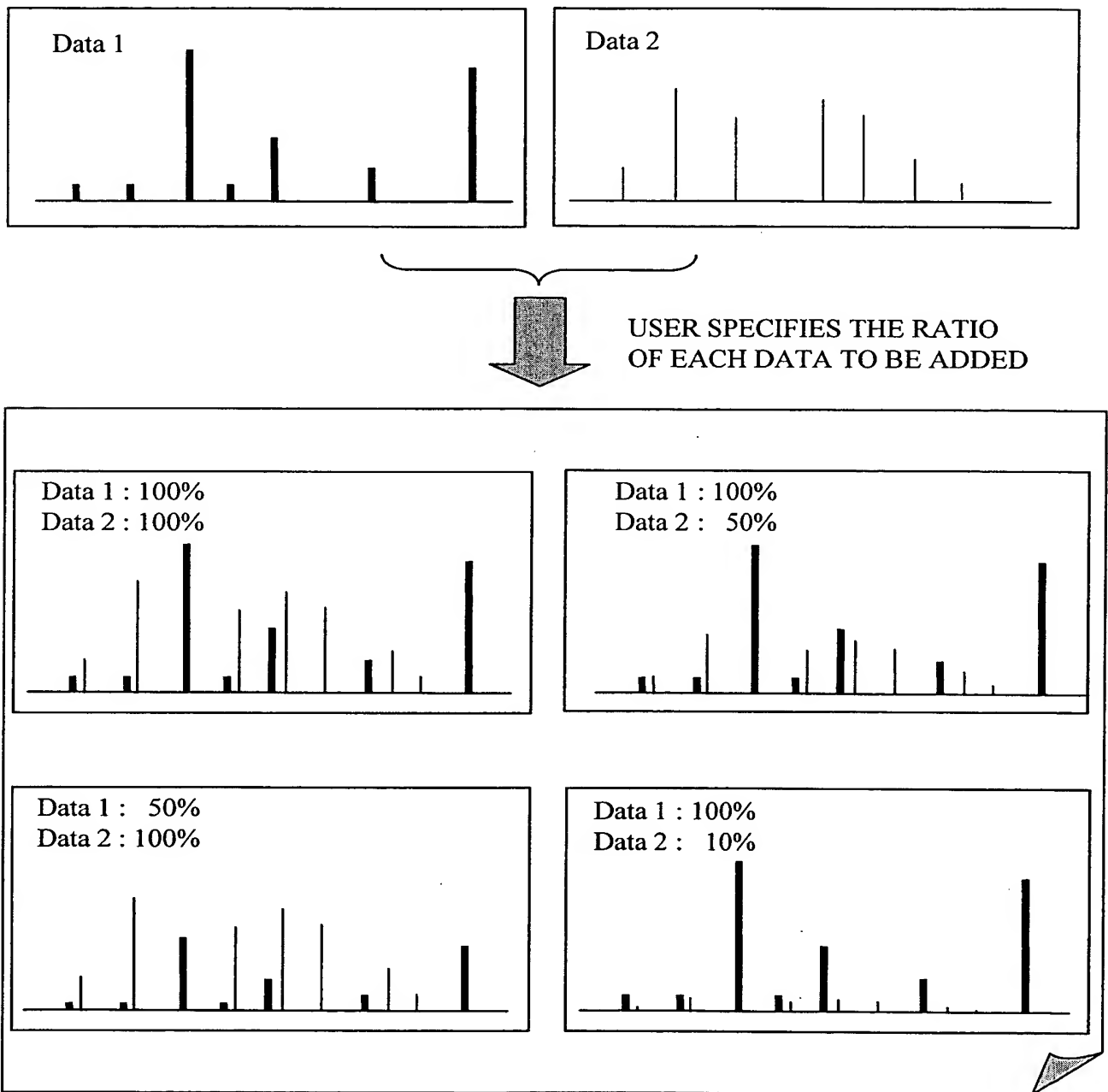


FIG. 34

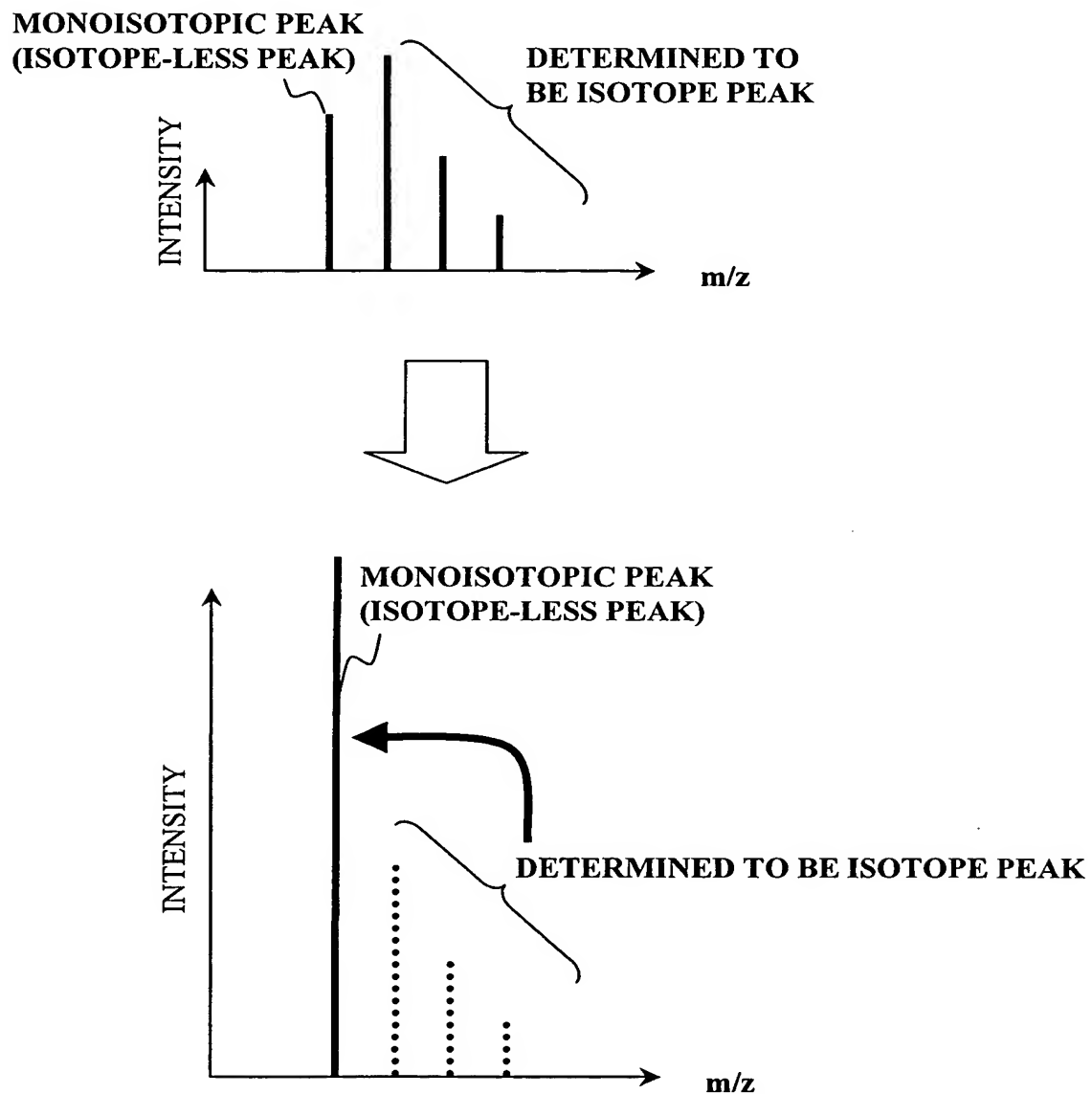


FIG. 35 a

PROTEIN ANALYSIS AND IDENTIFICATION FLOW IN PRIOR ART

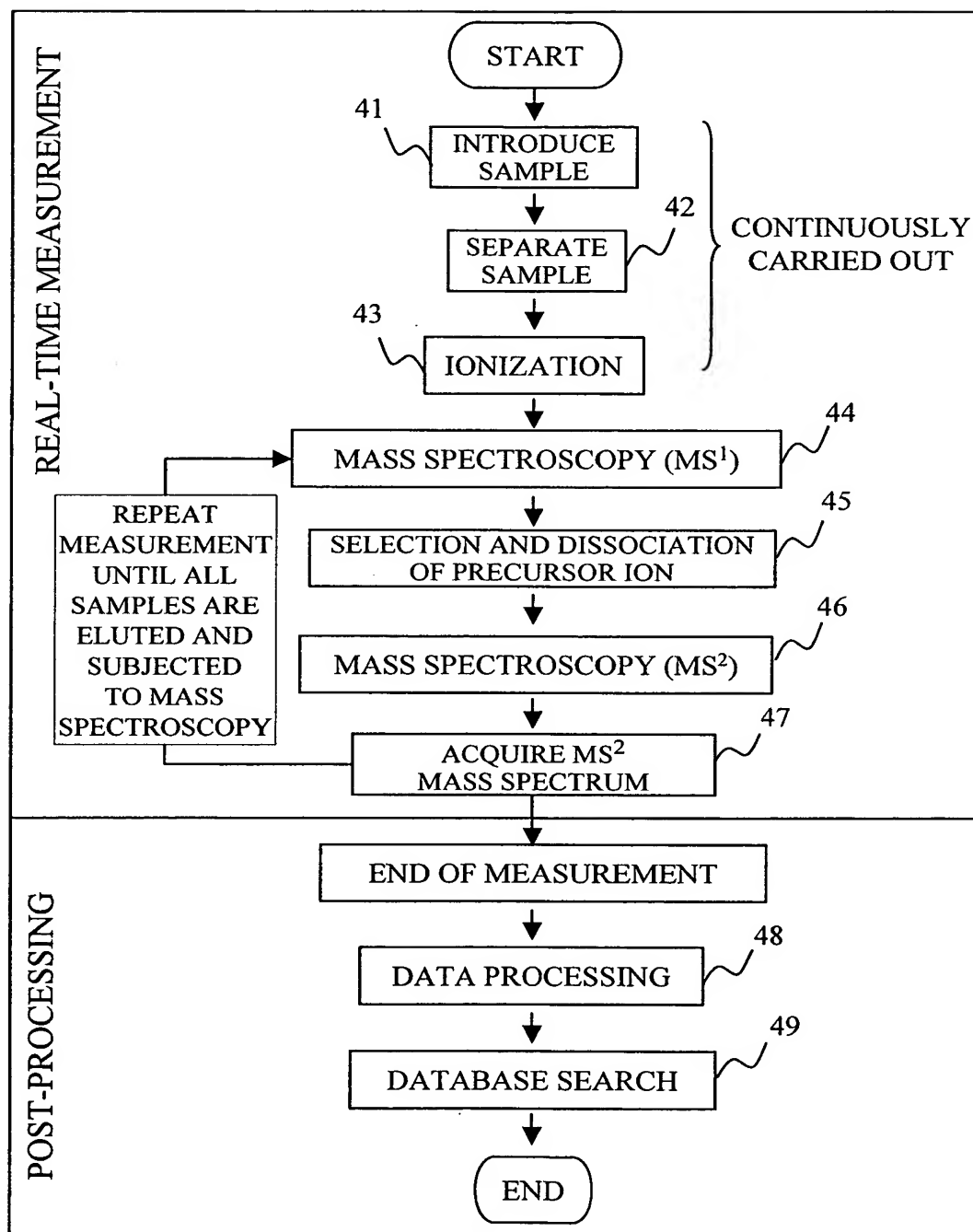


FIG. 35 b

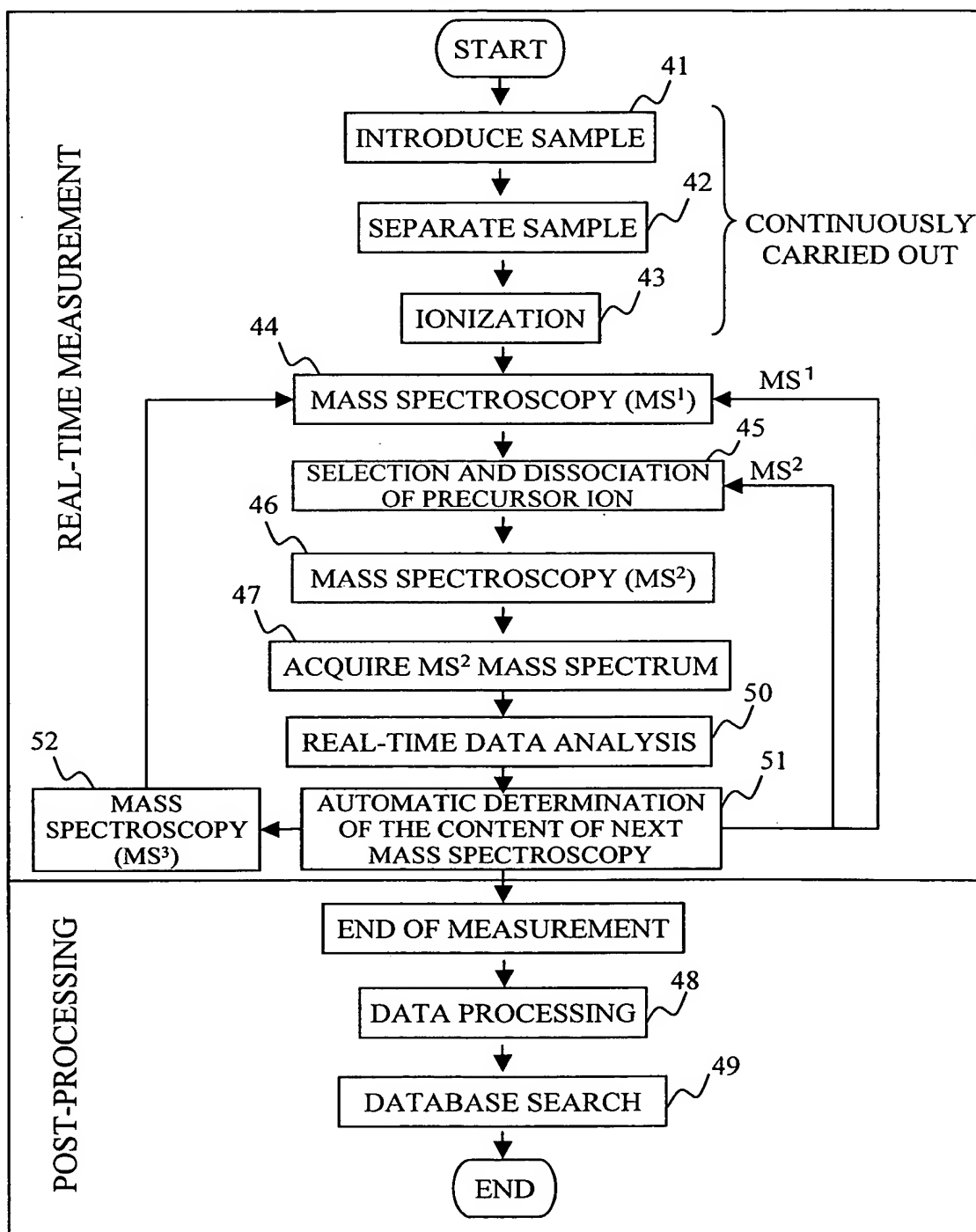
PROTEIN ANALYSIS AND IDENTIFICATION
FLOW IN THE PRESENT EMBODIMENT

FIG. 36

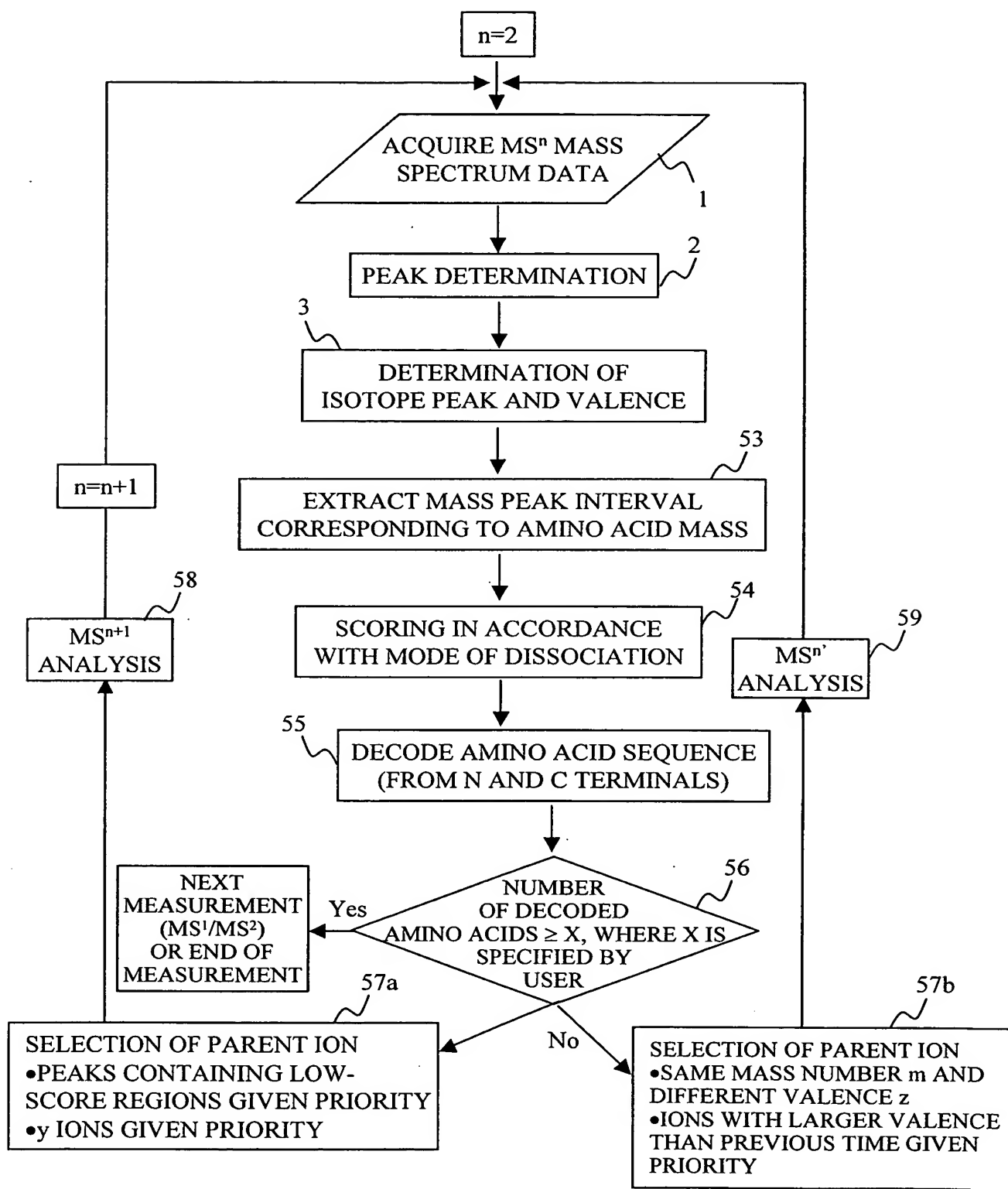
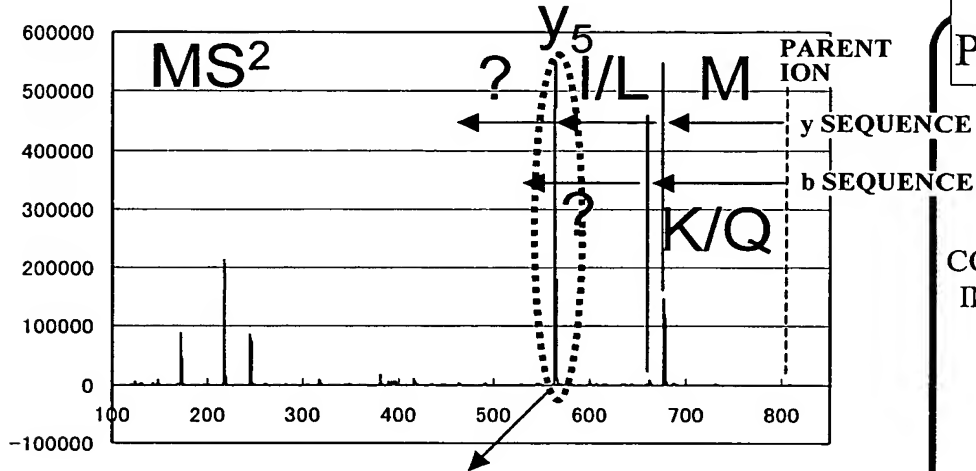


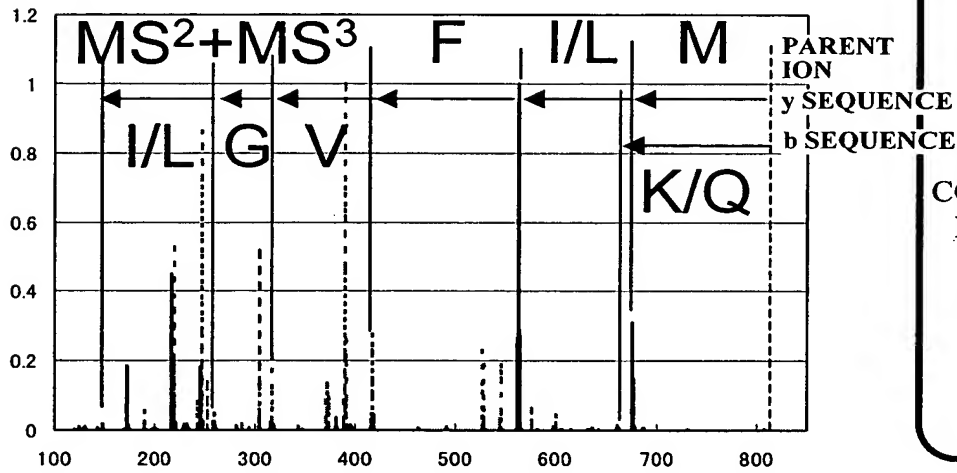
FIG. 37

MIFVGIK



m/z=563.2

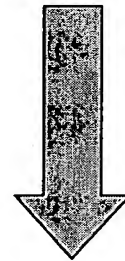
MS³ ANALYSIS PERFORMED



— MS² --- MS³

POST-PROCESSING

CORRECT SEQUENCE
 IN DB SEARCH: 10TH
 OR LOWER



CORRECT SEQUENCE
 IN DB SEARCH: 1ST

FIG. 38

FLOWCHART (REAL-TIME DB SEARCH)

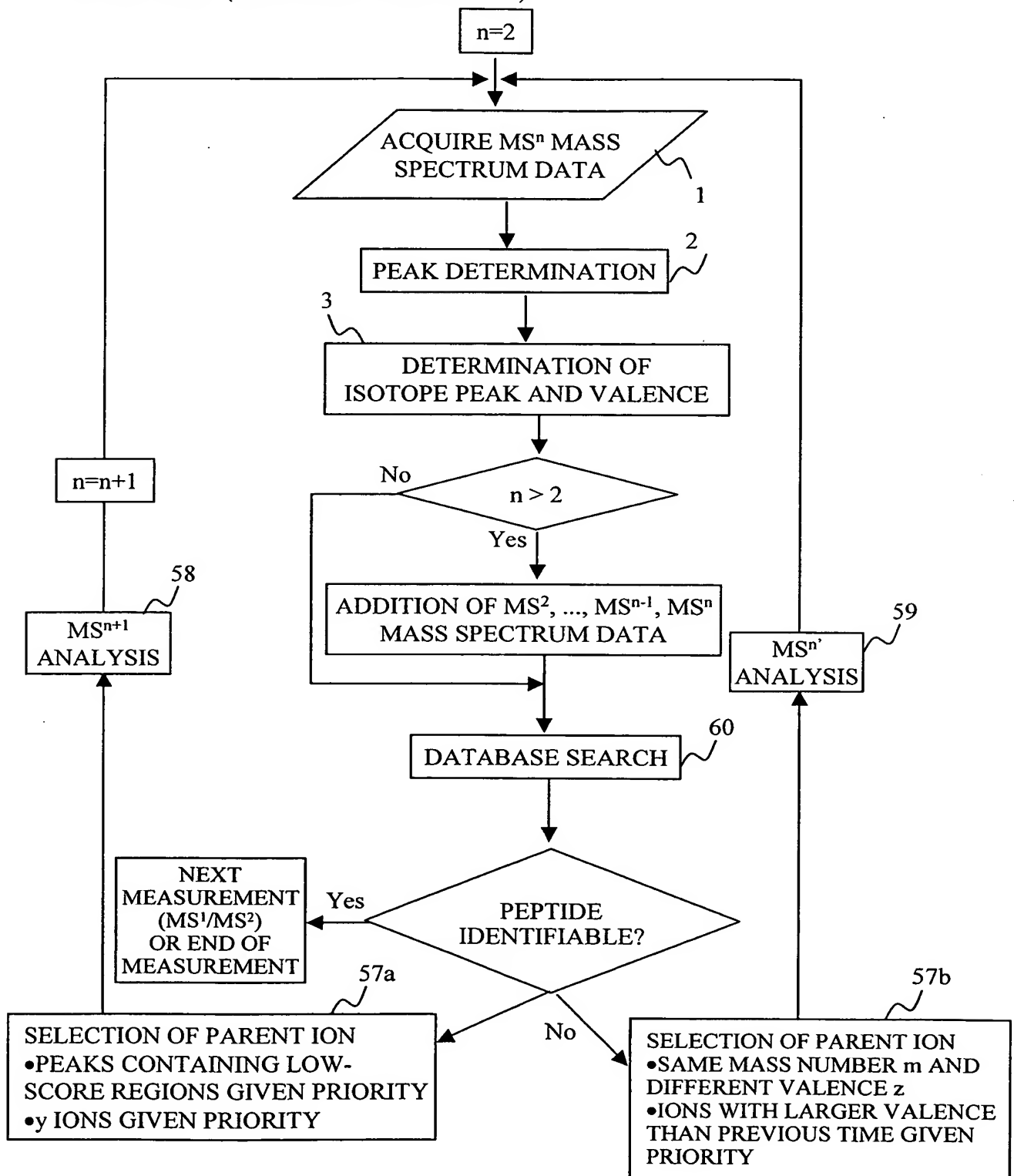


FIG. 39

(FLOWCHAR: SPECIFIC CONDITIONS → MS3/MS2')

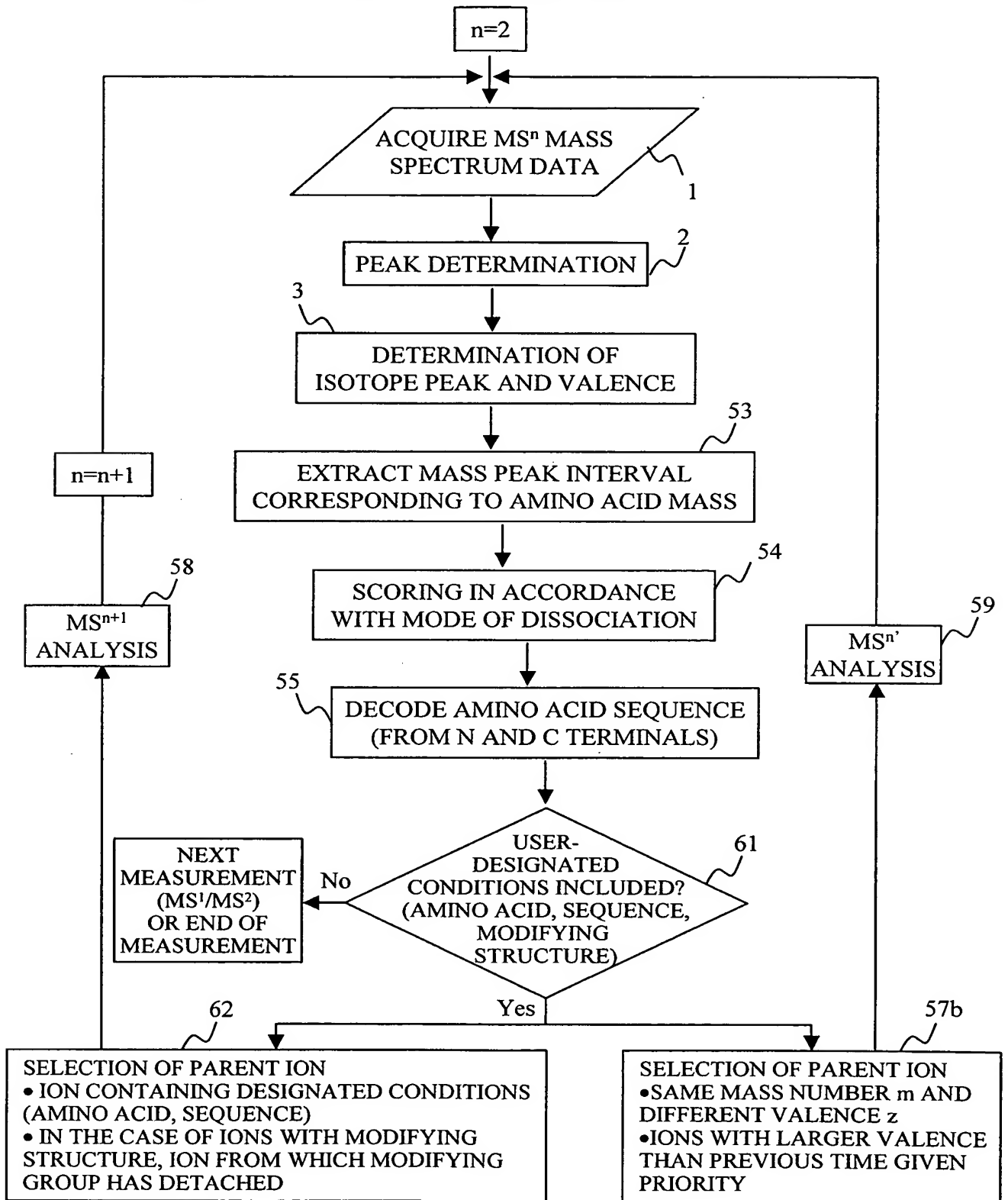


FIG. 40

(DERIVATION OF NUMBER OF PEAK GROUPS)

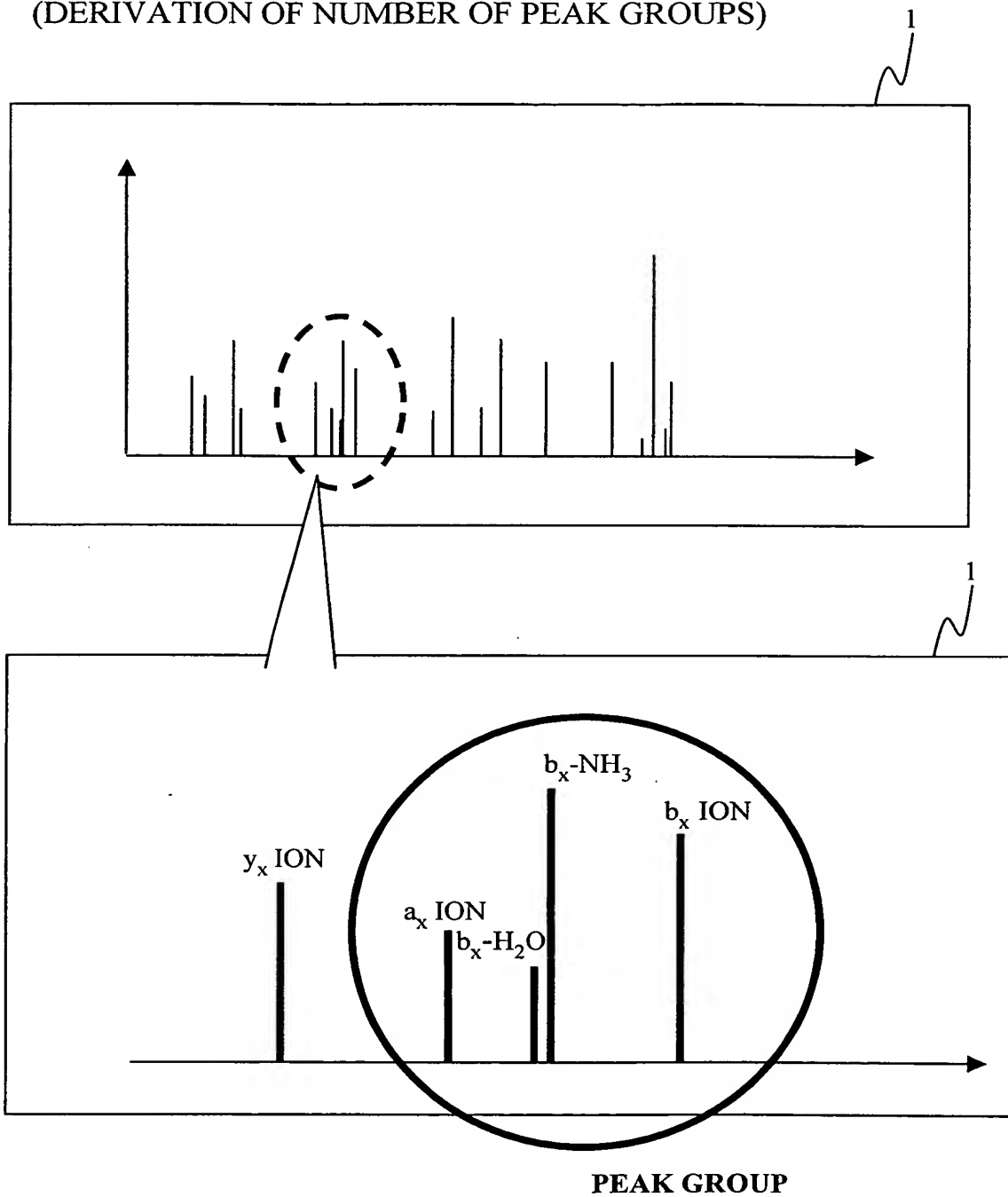


FIG. 41

(FLOWCHART: DETERMINATION BASED ON PEAK GROUP)

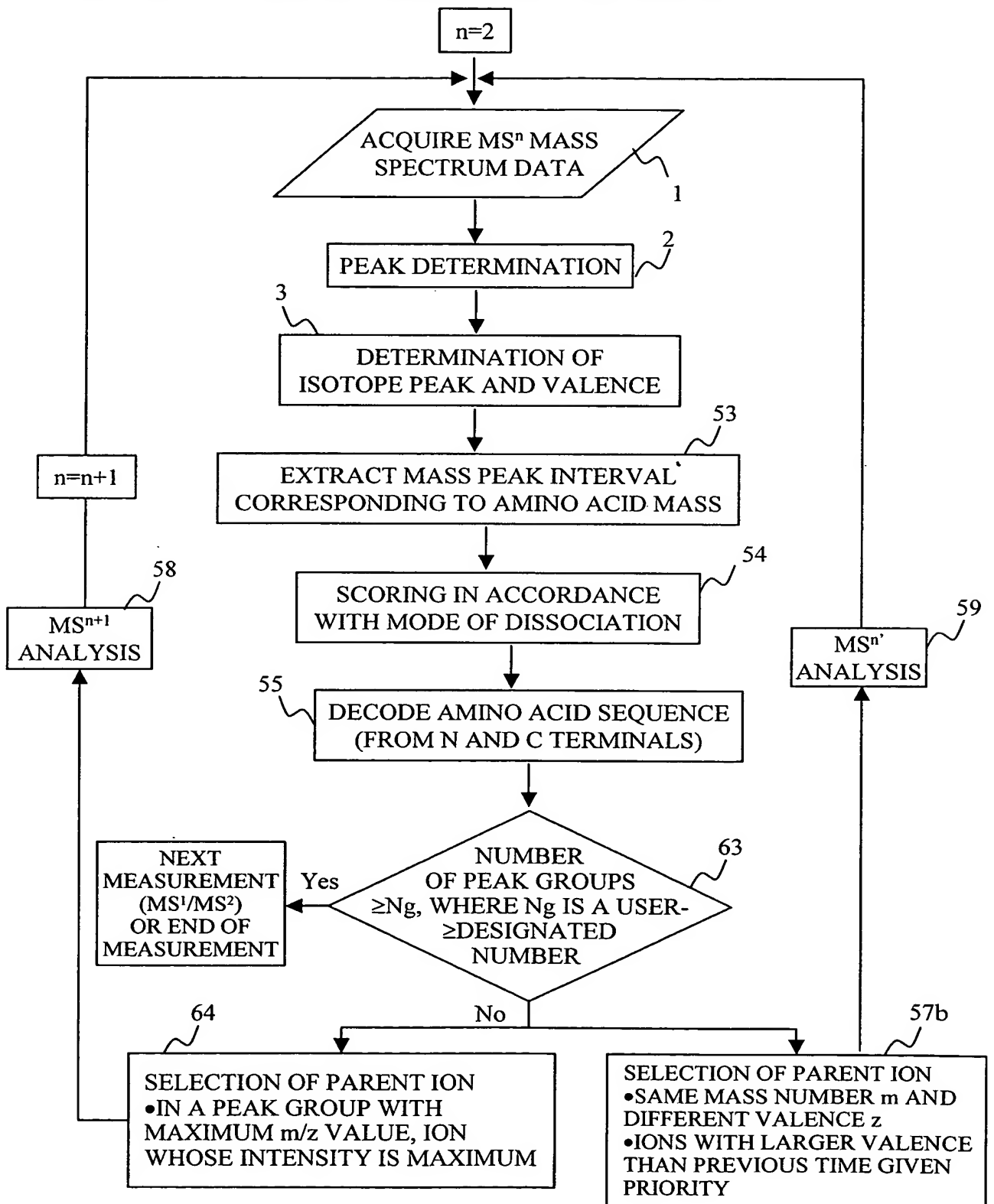


FIG. 42

(FLOWCHART: DETERMINATION BASED ON NUMBER OF PEAKS)

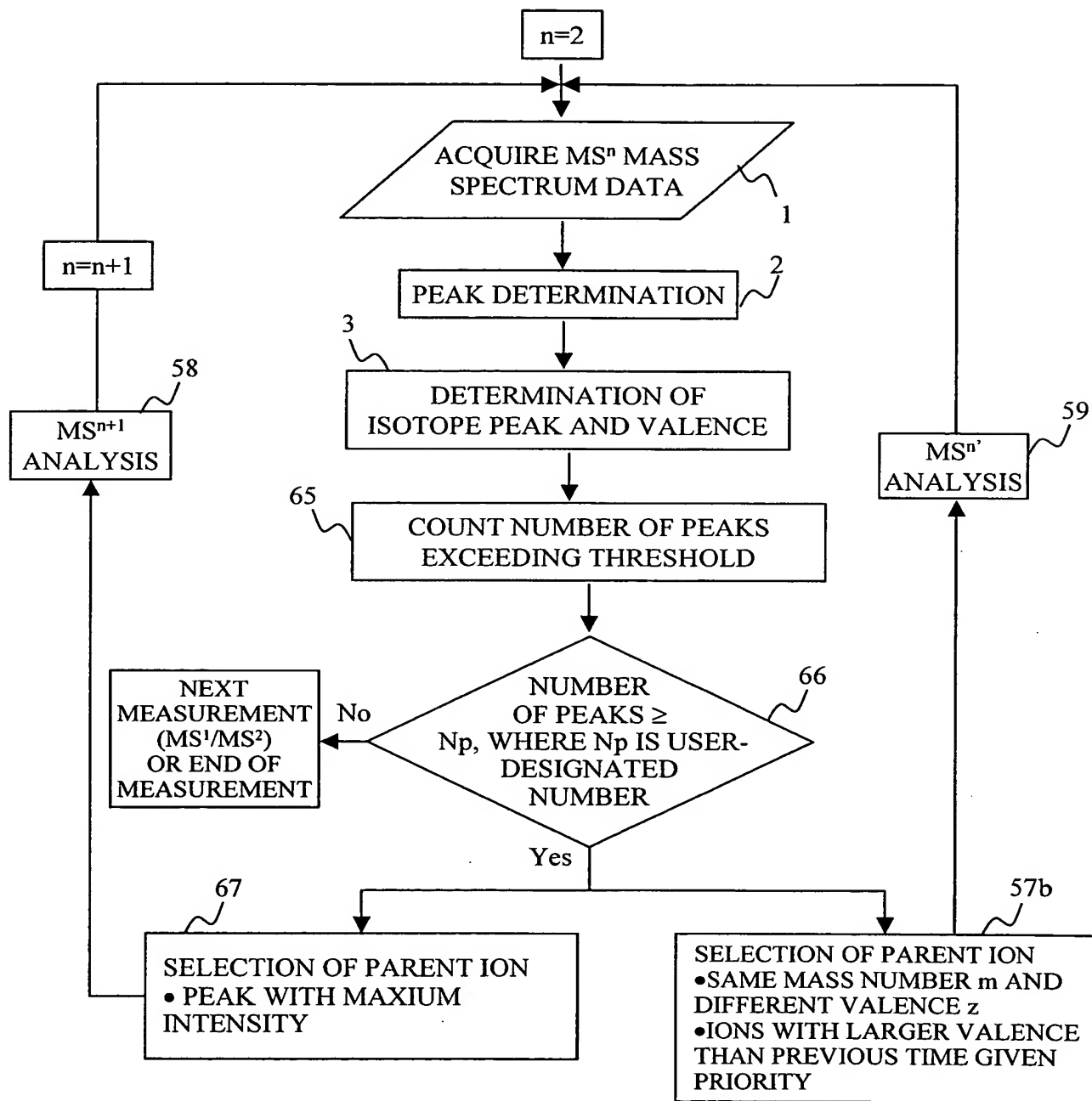


FIG. 43

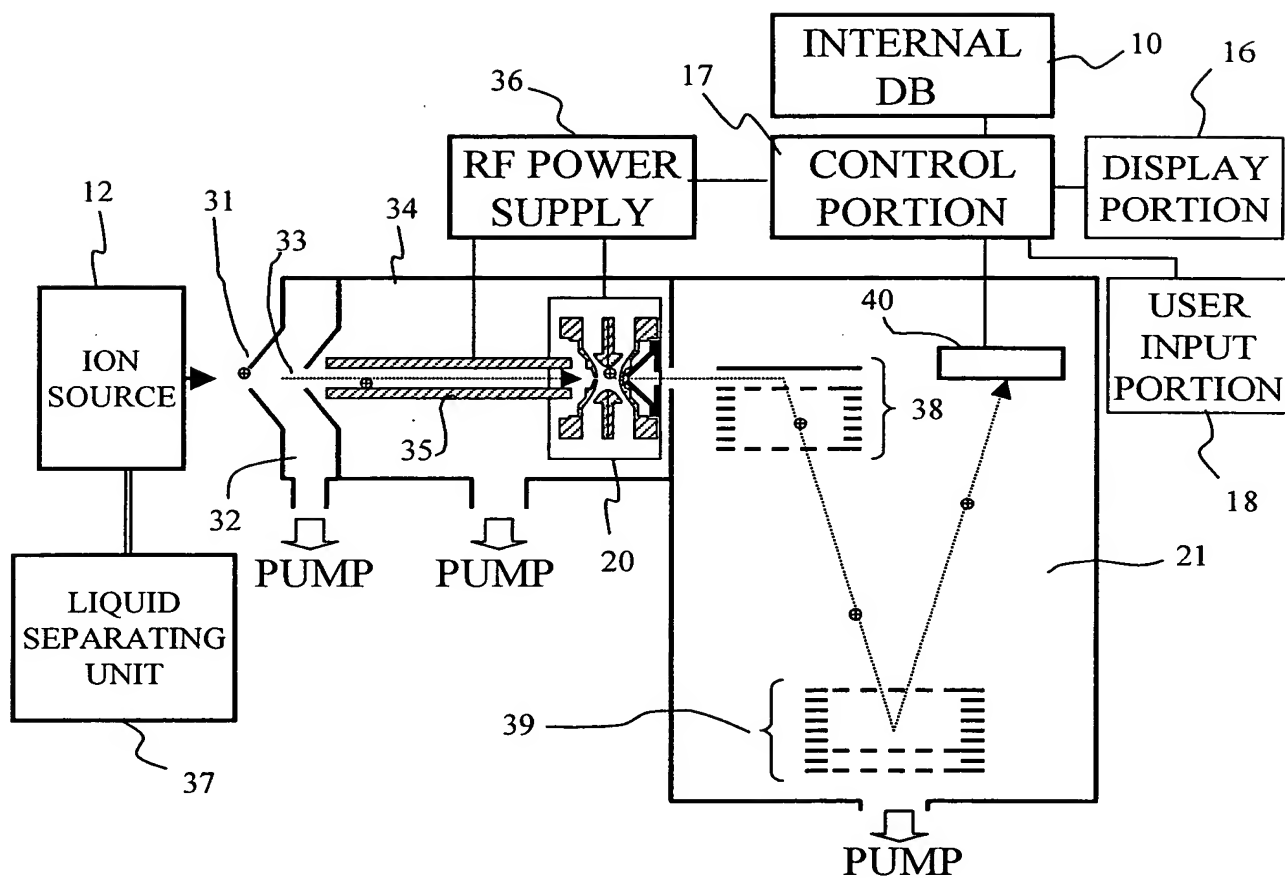


FIG. 44

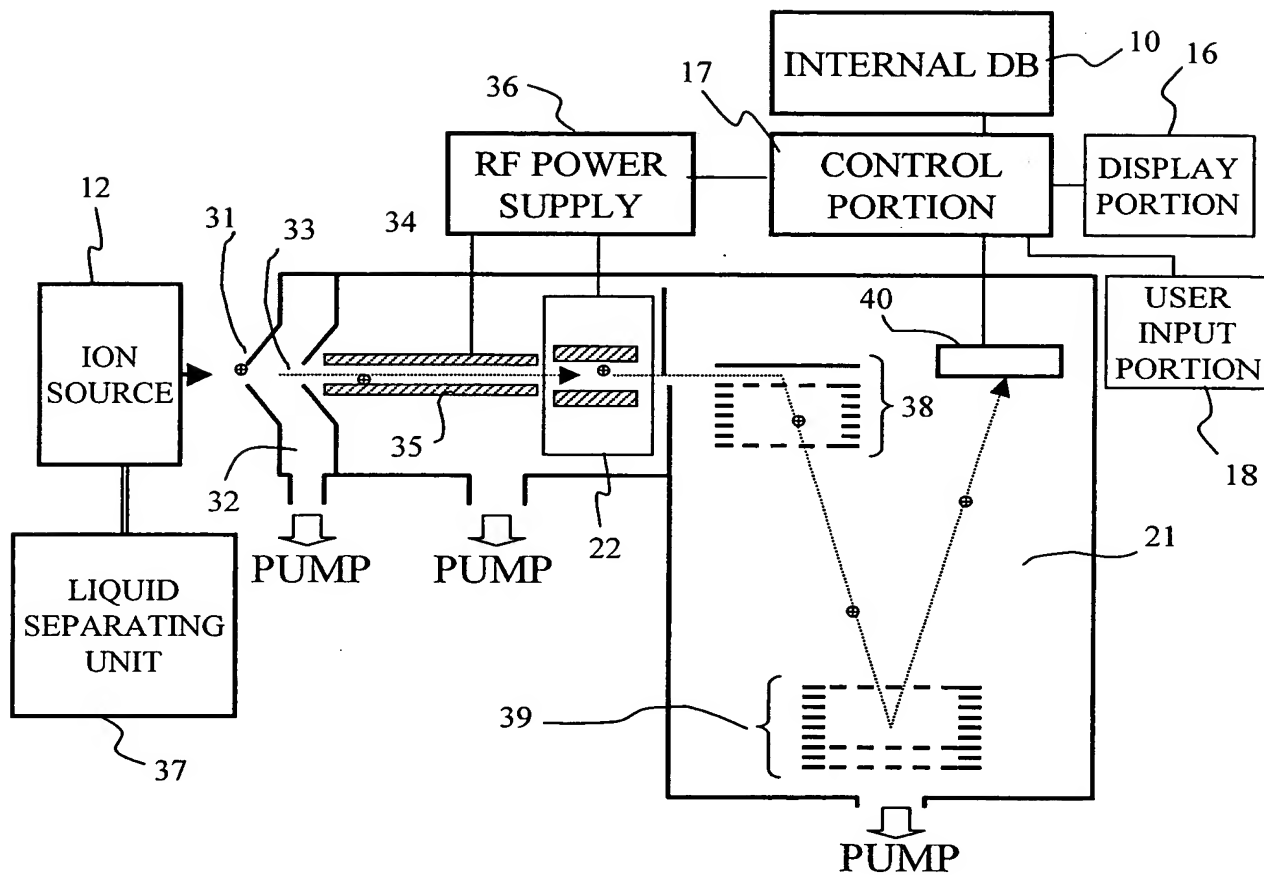


FIG. 45

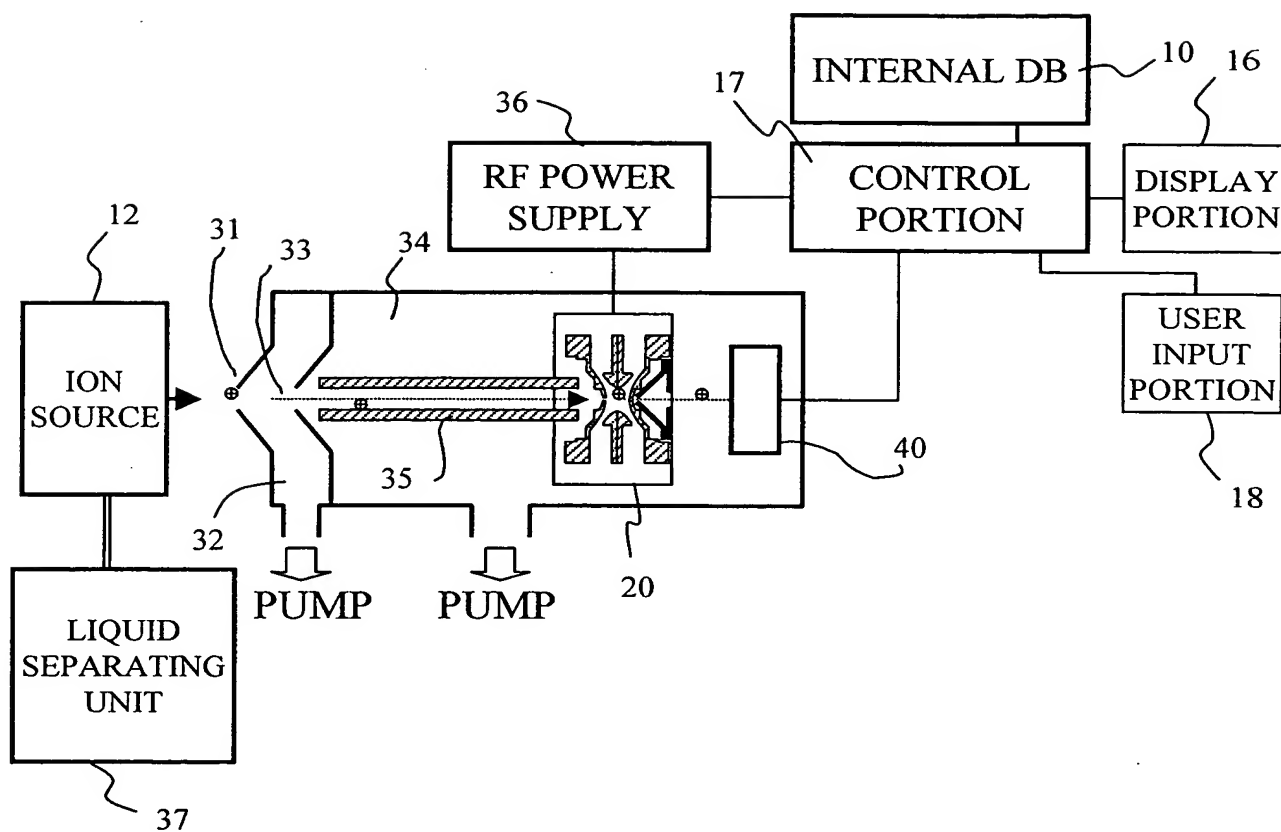


FIG. 46

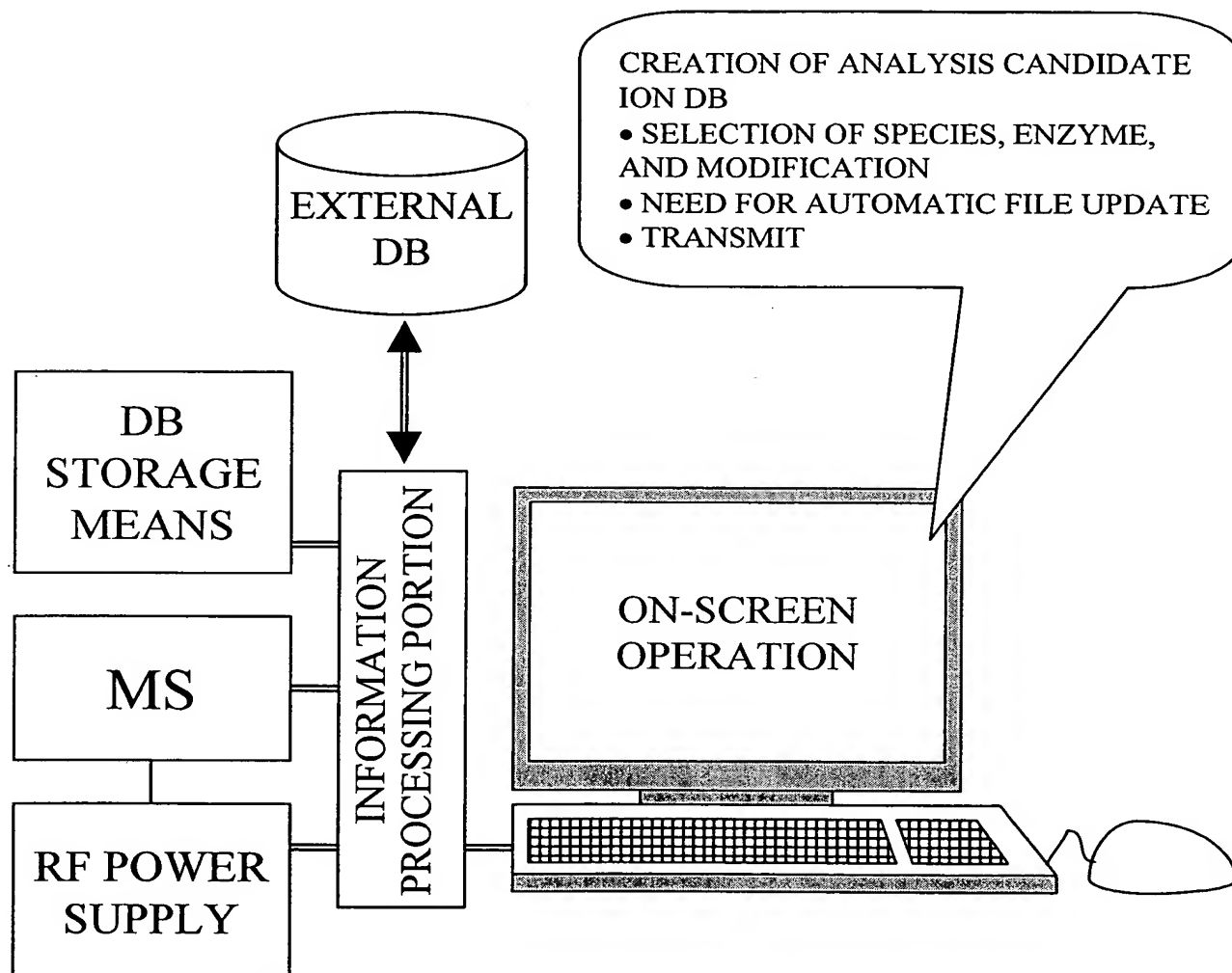


FIG. 47

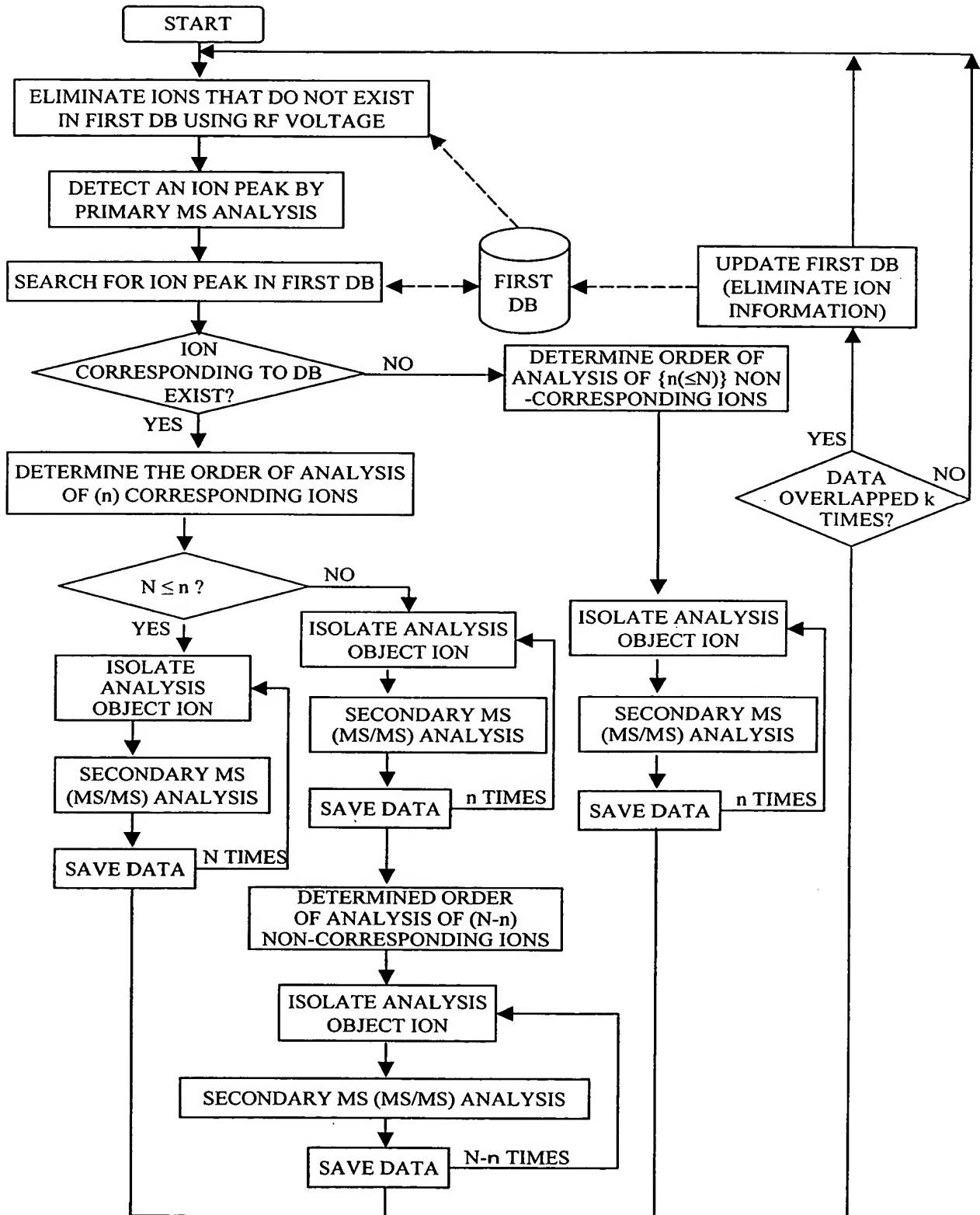


FIG. 48

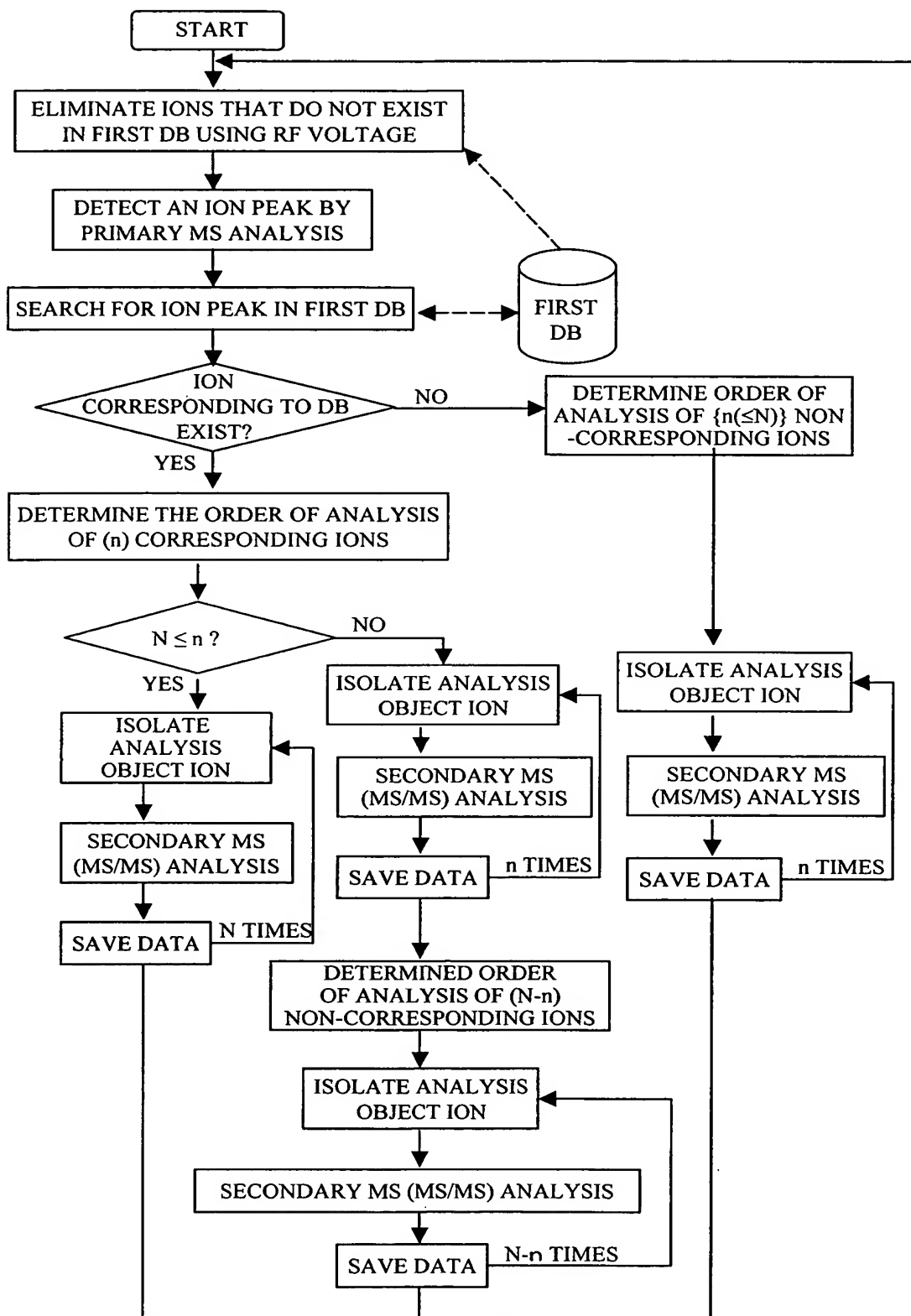


FIG. 49

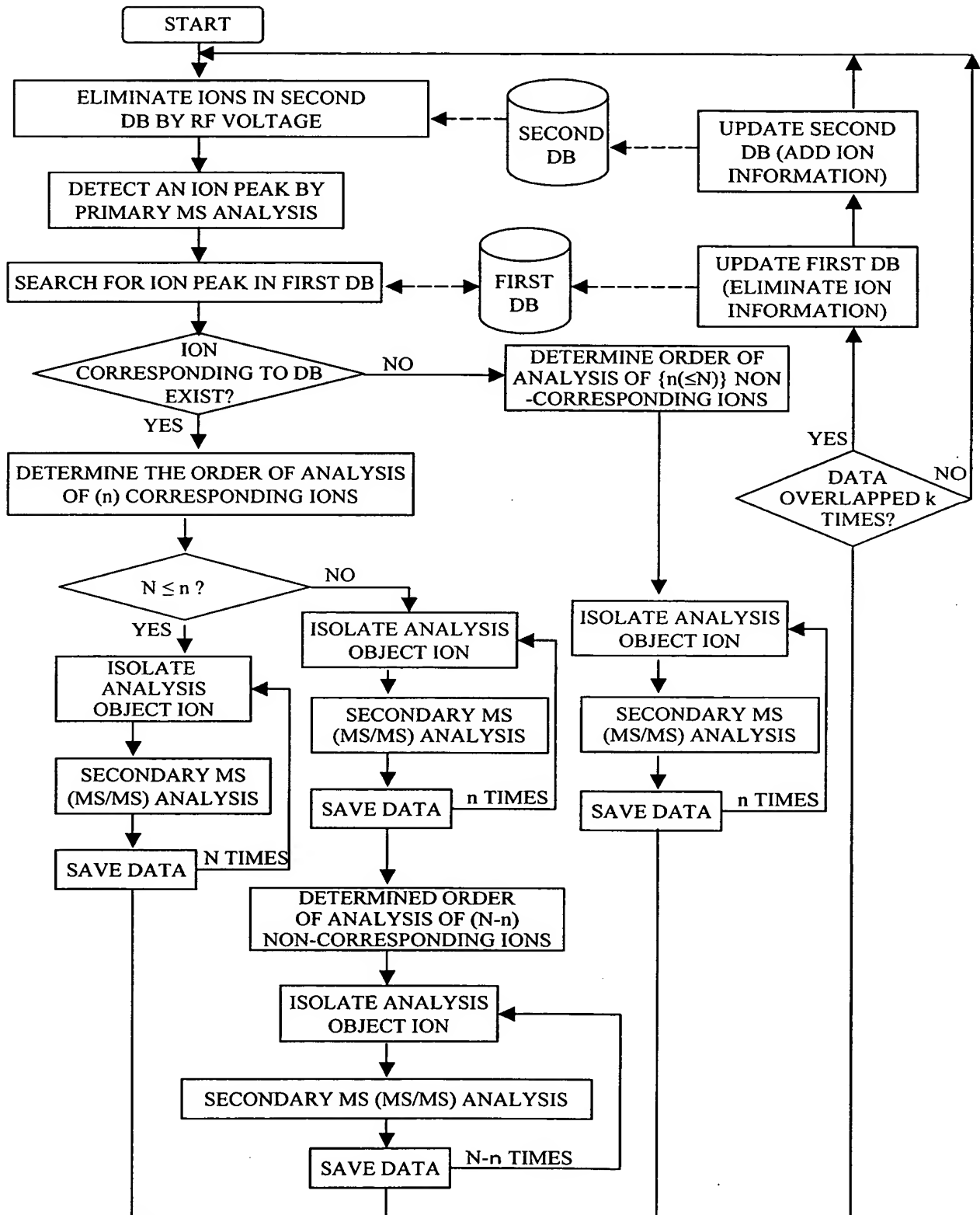


FIG. 50

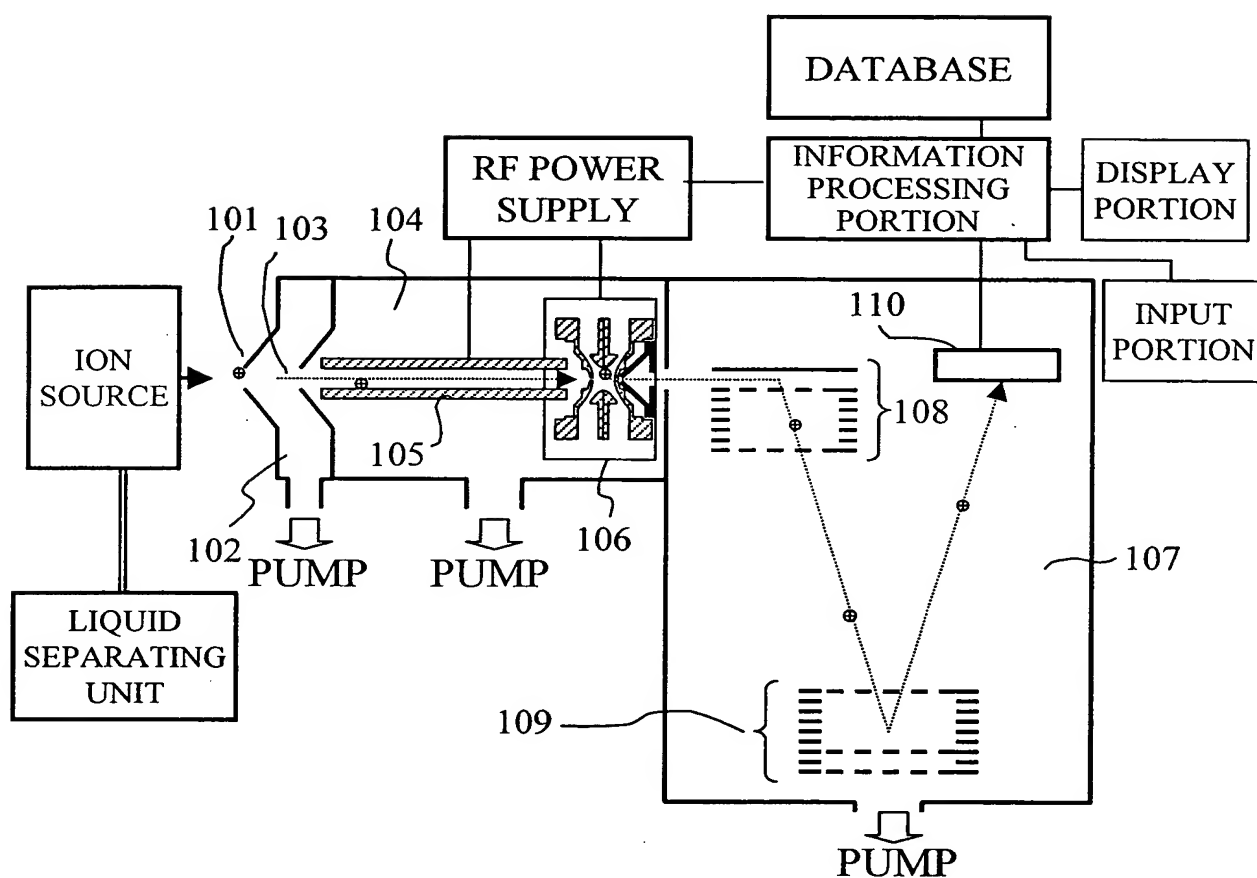


FIG. 51

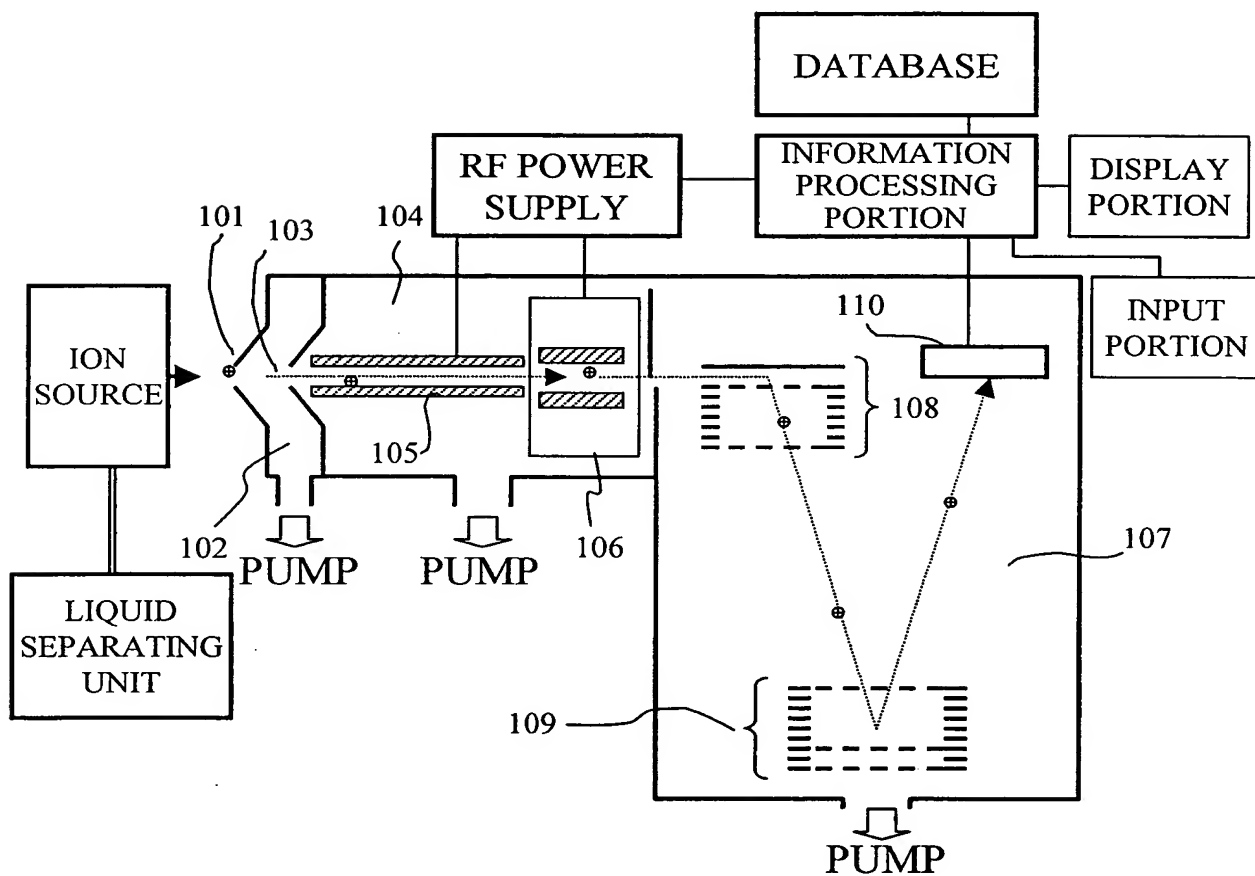
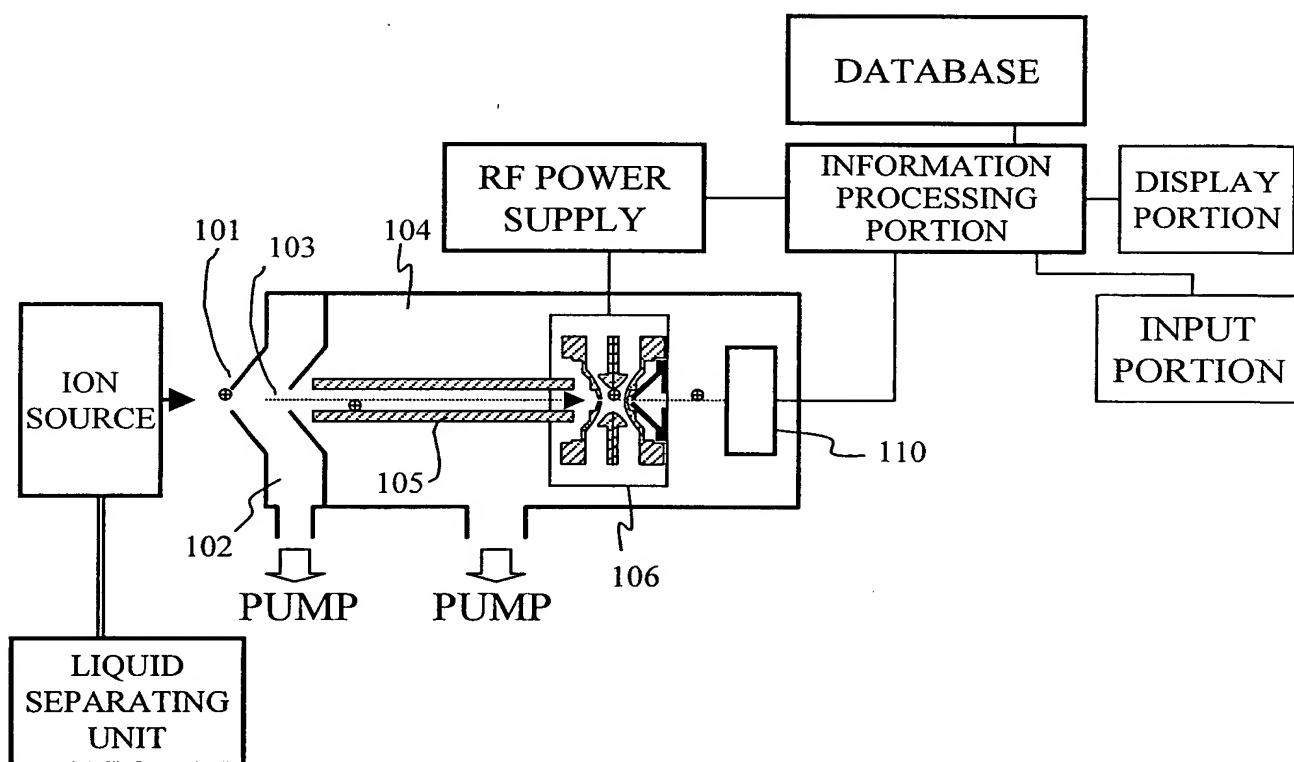


FIG. 52



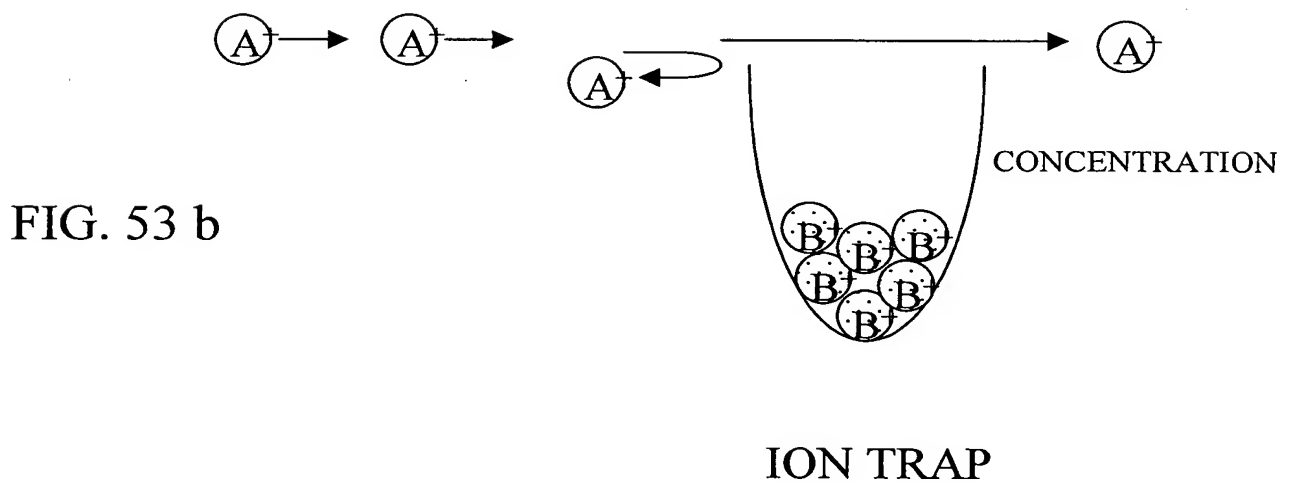
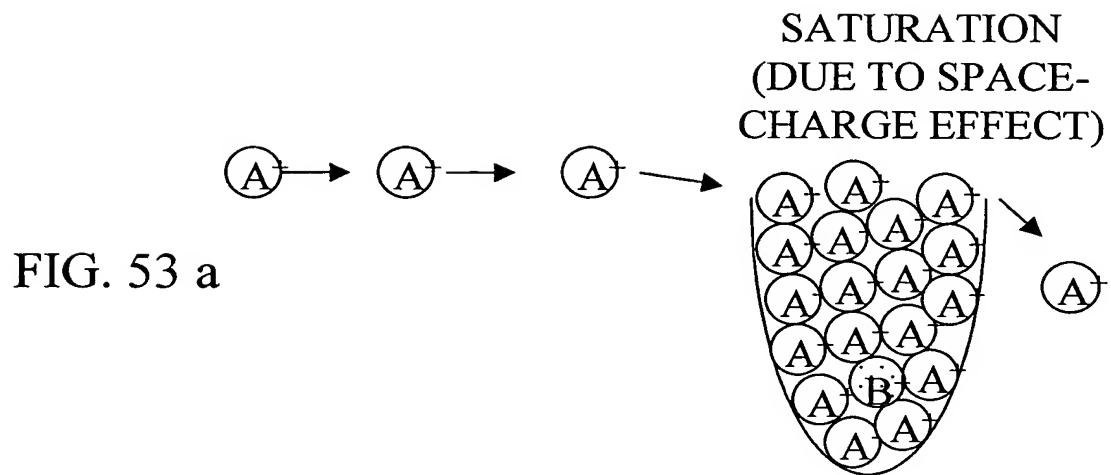


FIG. 54

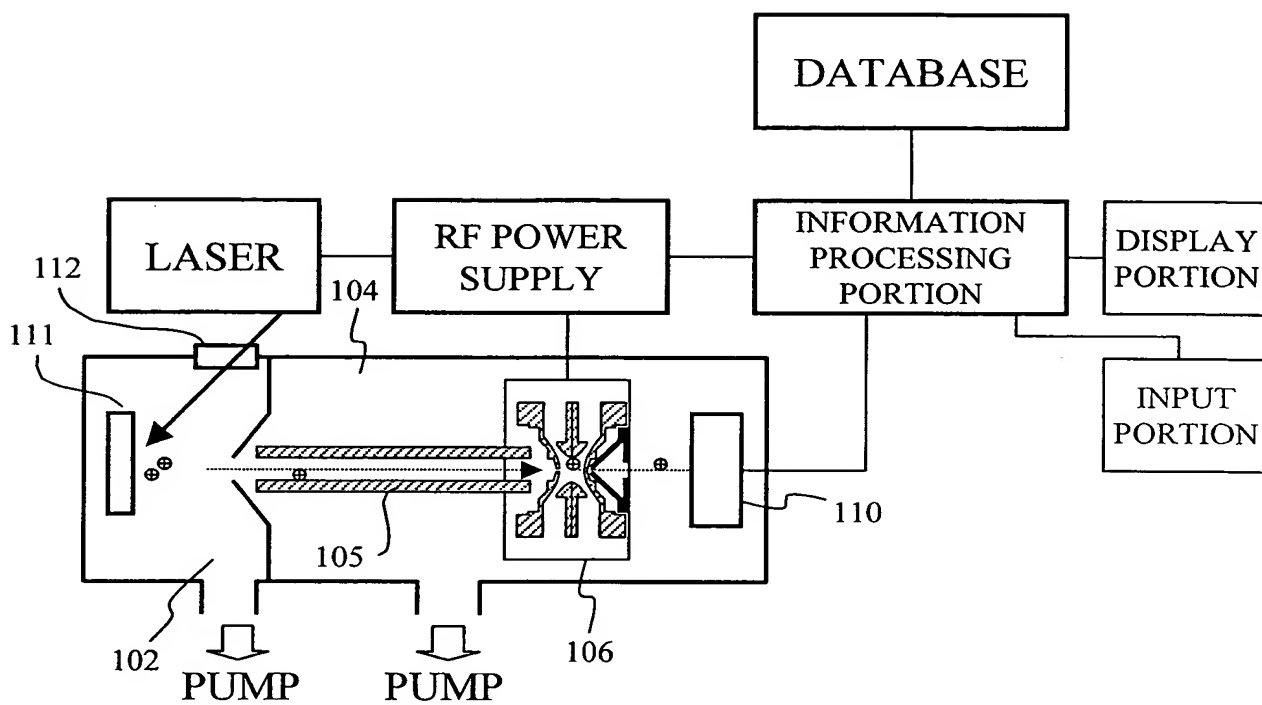


FIG. 55

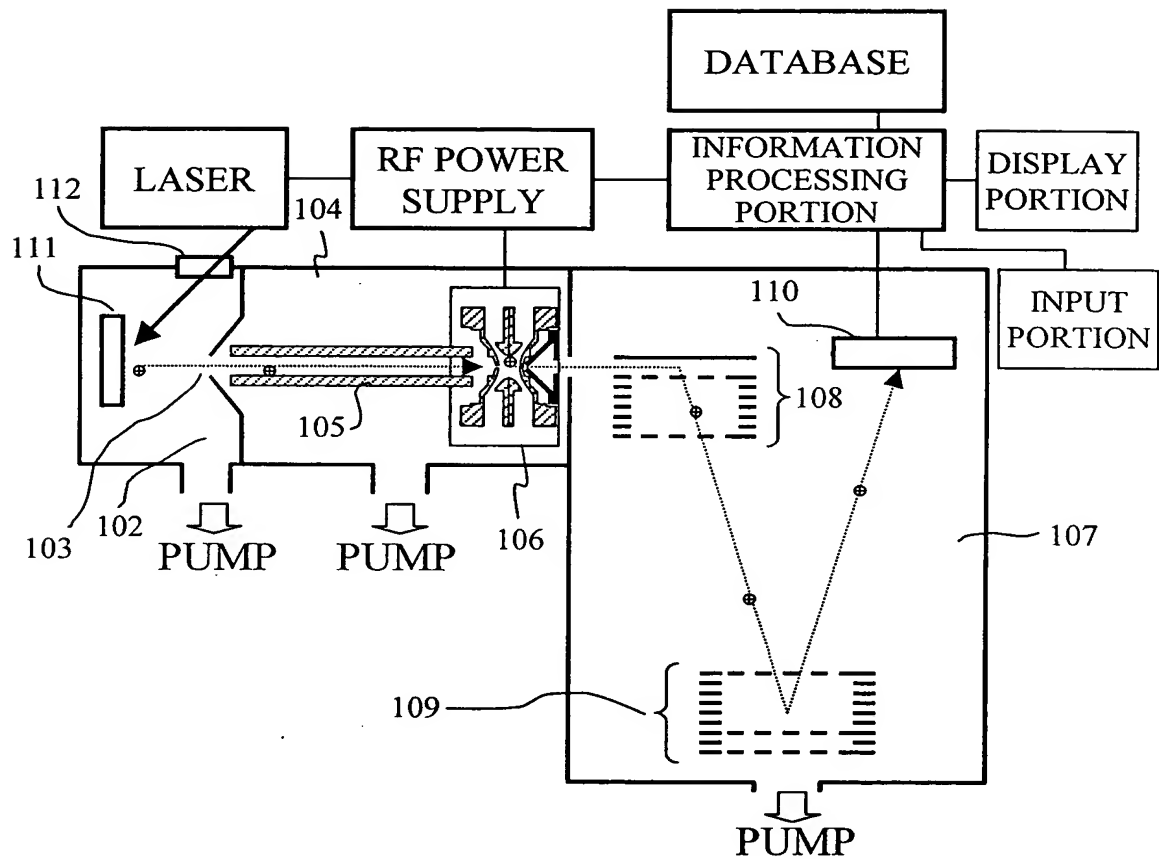


FIG. 56

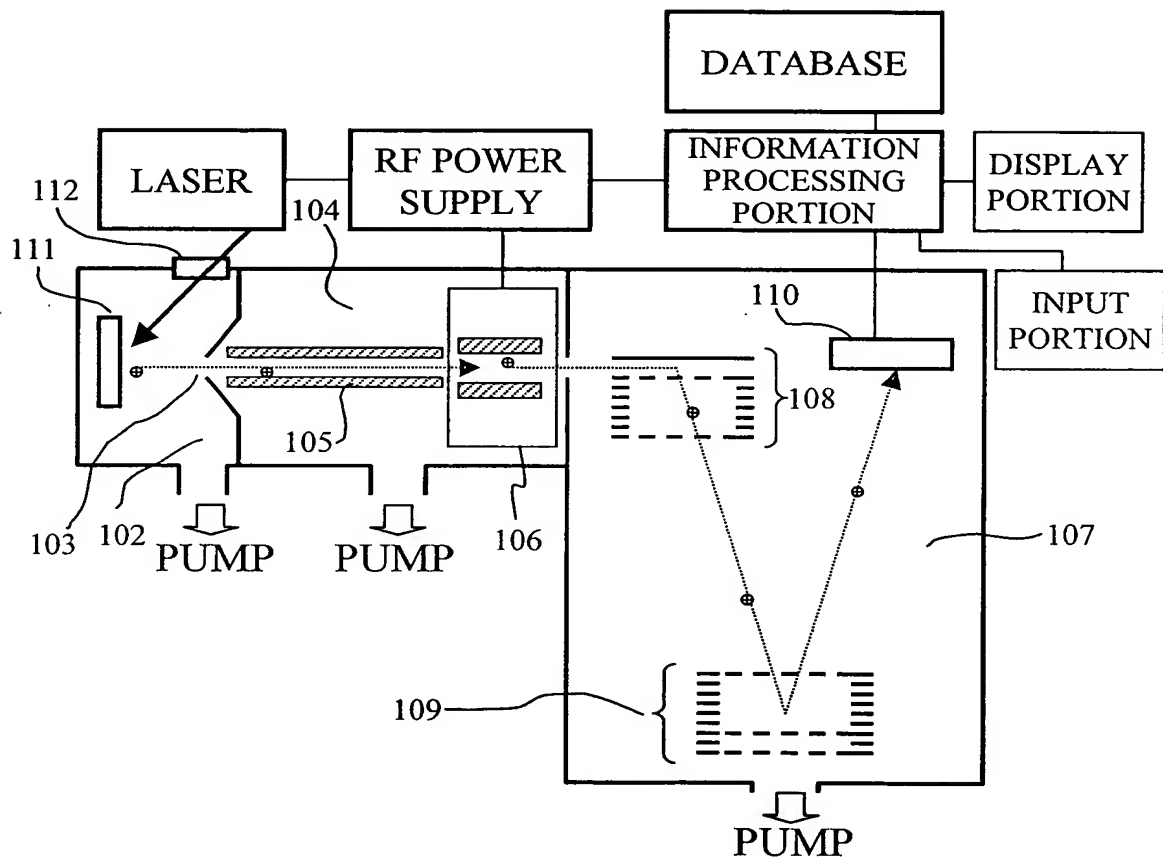


FIG. 57

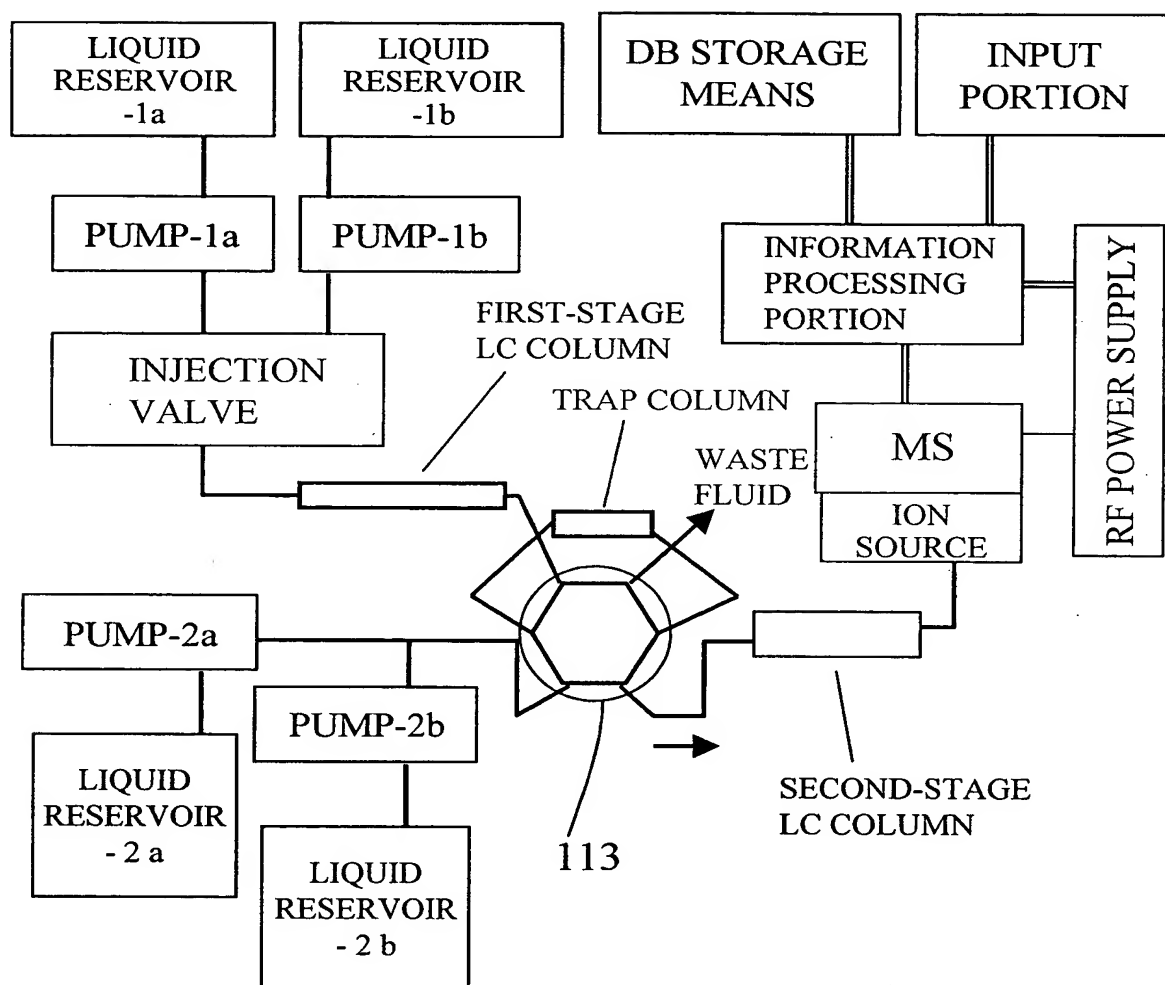


FIG. 58

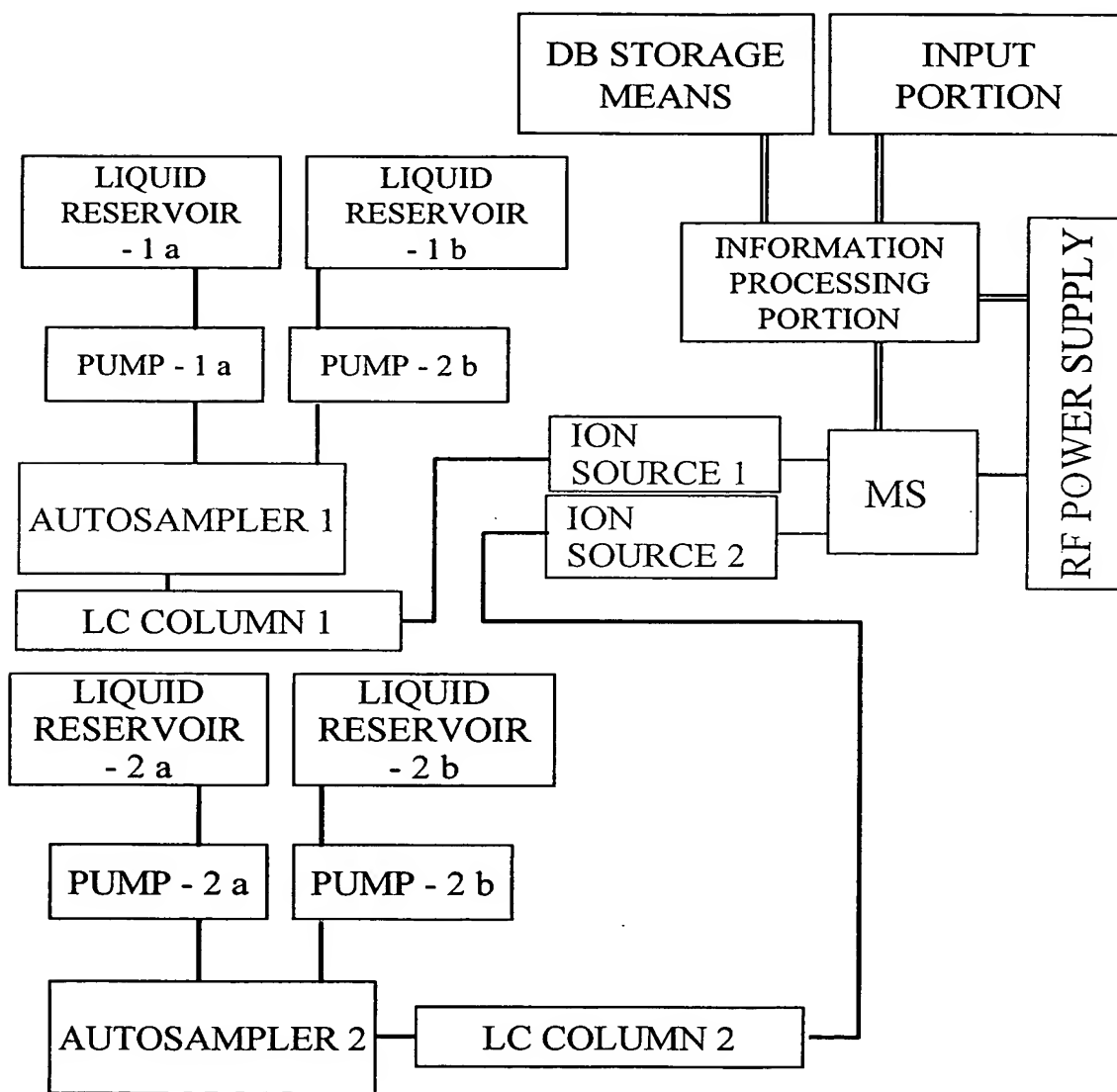


FIG. 59

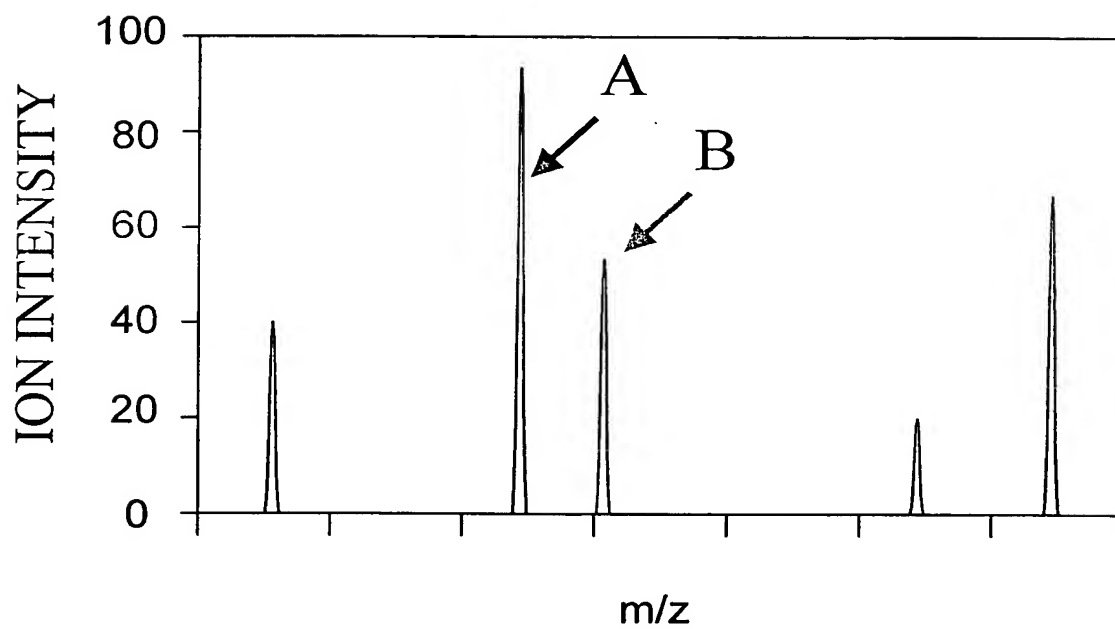
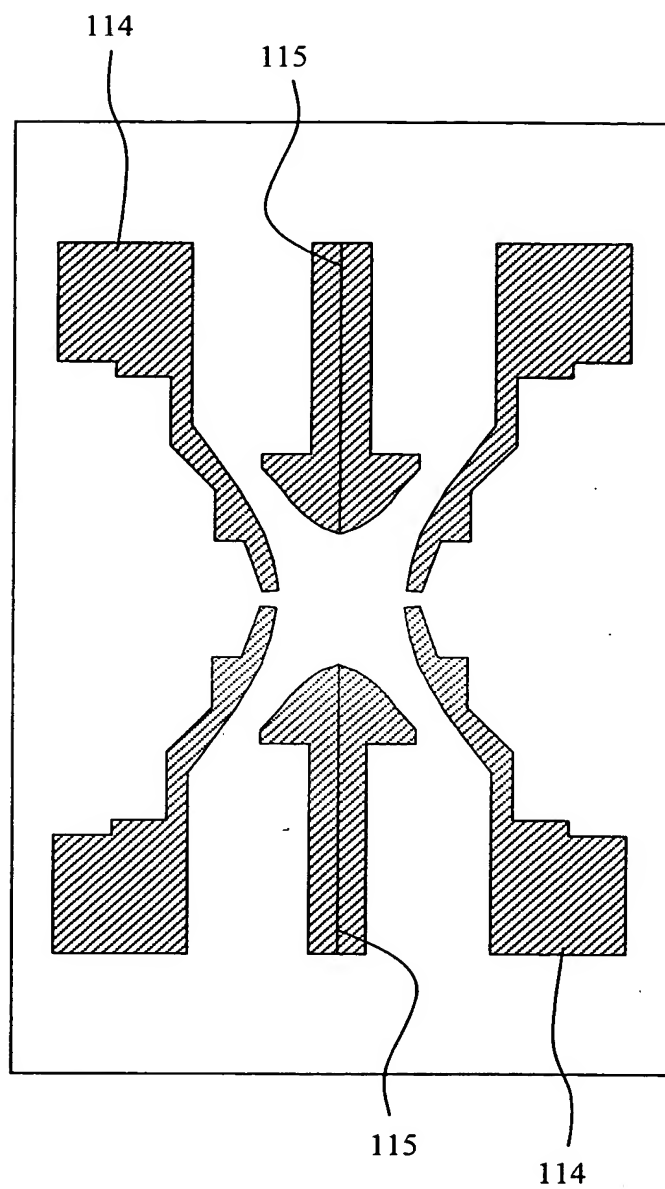


FIG. 60



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